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FIGURE 8A-1

HEADER GROWTH FACTOR
 TITLE HUMAN RECOMBINANT STEM CELL FACTOR 1SCF
 COMPND MOL_ID: 1;
 COMPND 2 MOLECULE: STEM CELL FACTOR;
 COMPND 3 CHAIN: A, B, C, D;
 COMPND 4 SYNONYM: SCF, SL, MGF, MAST CELL GROWTH FACTOR;
 COMPND 5 ENGINEERED: YES;
 COMPND 6 BIOLOGICAL_UNIT: DIMER
 SOURCE MOL_ID: 1;
 SOURCE 2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
 SOURCE 3 ORGANISM_COMMON: HUMAN;
 SOURCE 4 EXPRESSION_SYSTEM: NULL
 KEYWDS HUMAN STEM CELL FACTOR, STEEL FACTOR, KIT LIGAND, MAST CELL
 KEYWDS 2 GROWTH FACTOR
 EXPDTA X-RAY DIFFRACTION
 AUTHOR X.JIANG,O.GUREL,K.E.LANGLEY,W.A.HENDRICKSON
 JRNL AUTH X.JIANG,O.GUREL,K.E.LANGLEY,W.A.HENDRICKSON
 JRNL TITL CRYSTAL STRUCTURE OF RECOMBINANT HUMAN STEM CELL
 JRNL TITL 2 FACTOR
 JRNL REF TO BE PUBLISHED
 JRNL REFN 0353
 REMARK 1
 REMARK 2
 REMARK 2 RESOLUTION. 2.2 ANGSTROMS.
 REMARK 3
 REMARK 3 REFINEMENT.
 REMARK 3 PROGRAM : X-PLOR 3.1
 REMARK 3 AUTHORS : BRUNGER
 REMARK 3
 REMARK 3 DATA USED IN REFINEMENT.
 REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.2
 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 20.0
 REMARK 3 DATA CUTOFF (SIGMA(F)) : 2
 REMARK 3 DATA CUTOFF HIGH (ABS(F)) : 100000
 REMARK 3 DATA CUTOFF LOW (ABS(F)) : 0.1
 REMARK 3 COMPLETENESS (WORKING+TEST) (%) : 96.6
 REMARK 3 NUMBER OF REFLECTIONS : 49851
 REMARK 3
 REMARK 3 FIT TO DATA USED IN REFINEMENT.
 REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
 REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
 REMARK 3 R VALUE (WORKING SET) : 0.199
 REMARK 3 FREE R VALUE : 0.242
 REMARK 3 FREE R VALUE TEST SET SIZE (%) : 6.0
 REMARK 3 FREE R VALUE TEST SET COUNT : 3016
 REMARK 3 ESTIMATED ERROR OF FREE R VALUE : 0.0044
 REMARK 3
 REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
 REMARK 3 TOTAL NUMBER OF BINS USED : 10
 REMARK 3 BIN RESOLUTION RANGE HIGH (A) : 2.0
 REMARK 3 BIN RESOLUTION RANGE LOW (A) : 2.28
 REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 97.0
 REMARK 3 REFLECTIONS IN BIN (WORKING SET) : 4349
 REMARK 3 BIN R VALUE (WORKING SET) : 0.3159
 REMARK 3 BIN FREE R VALUE : 0.3450
 REMARK 3 BIN FREE R VALUE TEST SET SIZE (%) : 6.4
 REMARK 3 BIN FREE R VALUE TEST SET COUNT : 302
 REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.0198
 REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.

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FIGURE 8A-2

REMARK 3 PROTEIN ATOMS : 3517
REMARK 3 NUCLEIC ACID ATOMS : 0
REMARK 3 HETEROGEN ATOMS : 19
REMARK 3 SOLVENT ATOMS : 264
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : 38.5
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 32.1
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : NULL
REMARK 3 B22 (A**2) : NULL
REMARK 3 B33 (A**2) : NULL
REMARK 3 B12 (A**2) : NULL
REMARK 3 B13 (A**2) : NULL
REMARK 3 B23 (A**2) : NULL
REMARK 3
REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM LUZZATI PLOT (A) : NULL
REMARK 3 ESD FROM SIGMAA (A) : NULL
REMARK 3 LOW RESOLUTION CUTOFF (A) : NULL
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT (A) : NULL
REMARK 3 ESD FROM C-V SIGMAA (A) : NULL
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS (A) : 0.016
REMARK 3 BOND ANGLES (DEGREES) : 2.5
REMARK 3 DIHEDRAL ANGLES (DEGREES) : 22.8
REMARK 3 IMPROPER ANGLES (DEGREES) : 2.05
REMARK 3
REMARK 3 ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. RMS SIGMA
REMARK 3 MAIN-CHAIN BOND (A**2) : 1.2 ; 1.5
REMARK 3 MAIN-CHAIN ANGLE (A**2) : 1.6 ; 2.0
REMARK 3 SIDE-CHAIN BOND (A**2) : 2.1 ; 2.0
REMARK 3 SIDE-CHAIN ANGLE (A**2) : 2.4 ; 2.5
REMARK 3
REMARK 3 NCS MODEL : RESTRAINTS
REMARK 3
REMARK 3 NCS RESTRAINTS. RMS SIGMA/WEIGHT
REMARK 3 GROUP 1 POSITIONAL (A) : NULL ; NULL
REMARK 3 GROUP 1 B-FACTOR (A**2) : NULL ; NULL
REMARK 3
REMARK 3 PARAMETER FILE 1 : PARAM19_MOD.PRO
REMARK 3 PARAMETER FILE 2 : PARAM19_SOL
REMARK 3 PARAMETER FILE 3 : HETERO PARAM19.PAR
REMARK 3 TOPOLOGY FILE 1 : TOPH19_MOD.PRO
REMARK 3 TOPOLOGY FILE 2 : TOPH19_SOL
REMARK 3 TOPOLOGY FILE 3 : HETERO.TOP
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: REFINEMENT WAS PERFORMED WITH
REMARK 3 ANOMALOUS ON; PARAM19_MOD.PRO AND TOPH19_MOD.PRO ARE
REMARK 3 MODIFIED PARAMETER AND TOPOLOGY FILES OF PARAM19.PRO AND
REMARK 3 TOPH19.PRO, RESPECTIVELY, FOR SELENOMETHIONYL PROTEINS.
REMARK 3 NCS RESTRAINTS WERE APPLIED ONLY DURING THE INITIAL
REMARK 3 REFINEMENT.
REMARK 4
REMARK 4 1SCF COMPLIES WITH FORMAT V. 2.3,

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FIGURE 8A-3

REMARK 6
REMARK 6 THE FOLLOWING RESIDUES ARE DISORDERED IN THE STRUCTURE:
REMARK 6 A1-10; A92-103; B1-10; B130-136; B139-141; C1-10; C92-103;
REMARK 6 C127-141; D1-10; D91-103; D128-141
REMARK 7
REMARK 7 THE SIDE CHAINS OF THE FOLLOWING RESIDUES ARE DISORDERED IN
REMARK 7 THE STRUCTURE: A11-13,A91,A127,A133,B11,B13,B93,B96-97,
REMARK 7 B103,B128,B137,C11,C13,C39,D11,D13,D90,D106,D127
REMARK 8
REMARK 8 LYS A 91 IS LAST RESIDUE BEFORE GAP, PHE B 129 IS LAST
REMARK 8 RESIDUE BEFORE GAP, LYS C 91 IS LAST RESIDUE BEFORE GAP,
REMARK 8 PHE C 126 IS LAST RESIDUE BEFORE GAP, VAL D 90 IS LAST
REMARK 8 RESIDUE BEFORE GAP.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION :
REMARK 200 TEMPERATURE (KELVIN) : 110
REMARK 200 PH : 7.4
REMARK 200 NUMBER OF CRYSTALS USED : 1
REMARK 200
REMARK 200 SYNCHROTRON (Y/N) : Y
REMARK 200 RADIATION SOURCE : NSLS
REMARK 200 BEAMLINE : X4A
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A) : 0.986
REMARK 200 MONOCHROMATOR : SILICON CRYSTAL
REMARK 200 OPTICS : MIRRORS
REMARK 200
REMARK 200 DETECTOR TYPE : IMAGE PLATE
REMARK 200 DETECTOR MANUFACTURER : FUJI
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENSO
REMARK 200 DATA SCALING SOFTWARE : SCALEPACK
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 65689
REMARK 200 RESOLUTION RANGE HIGH (A) : 2.0
REMARK 200 RESOLUTION RANGE LOW (A) : 25
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : -3
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE (%) : 94.9
REMARK 200 DATA REDUNDANCY : 2.75
REMARK 200 R MERGE (I) : NULL
REMARK 200 R SYM (I) : 0.056
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 15.3
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.0
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : 2.07
REMARK 200 COMPLETENESS FOR SHELL (%) : 72
REMARK 200 DATA REDUNDANCY IN SHELL : 2.23
REMARK 200 R MERGE FOR SHELL (I) : NULL
REMARK 200 R SYM FOR SHELL (I) : 0.581
REMARK 200 <I/SIGMA(I)> FOR SHELL : 1.6
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: NULL
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD
REMARK 200 SOFTWARE USED: MADLSQ
REMARK 200 STARTING MODEL: NULL

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FIGURE 8A-4

REMARK 200
 REMARK 200 REMARK: NULL
 REMARK 280
 REMARK 280 CRYSTAL
 REMARK 280 SOLVENT CONTENT, VS (%): NULL
 REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
 REMARK 280
 REMARK 280 CRYSTALLIZATION CONDITIONS: PROTEIN WAS CRYSTALLIZED FROM
 REMARK 280 22% PEG 400, 220 MM CACL2, 100 MM HEPES, PH 7.4 AND 5MM
 REMARK 280 DTT IN 20 DEGREE ROOM
 REMARK 290
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
 REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 21
 REMARK 290
 REMARK 290 SYMOP SYMMETRY
 REMARK 290 NNNMMM OPERATOR
 REMARK 290 1555 X,Y,Z
 REMARK 290 2555 1/2-X,-Y,1/2+Z
 REMARK 290 3555 -X,1/2+Y,1/2-Z
 REMARK 290 4555 1/2+X,1/2-Y,-Z
 REMARK 290
 REMARK 290 WHERE NNN -> OPERATOR NUMBER
 REMARK 290 MMM -> TRANSLATION VECTOR
 REMARK 290
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
 REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
 REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
 REMARK 290 RELATED MOLECULES.
 REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 0.000000
 REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.000000
 REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.000000
 REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 35.90922
 REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000 0.000000
 REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 44.09560
 REMARK 290 SMTRY1 3 -1.000000 0.000000 0.000000 0.000000
 REMARK 290 SMTRY2 3 0.000000 1.000000 0.000000 41.27456
 REMARK 290 SMTRY3 3 0.000000 0.000000 -1.000000 44.09560
 REMARK 290 SMTRY1 4 1.000000 0.000000 0.000000 35.90922
 REMARK 290 SMTRY2 4 0.000000 -1.000000 0.000000 41.27456
 REMARK 290 SMTRY3 4 0.000000 0.000000 -1.000000 0.000000
 REMARK 290
 REMARK 290 REMARK: NULL
 REMARK 295
 REMARK 295 NON-CRYSTALLOGRAPHIC SYMMETRY
 REMARK 295 THE TRANSFORMATIONS PRESENTED ON THE MTRIX RECORDS BELOW
 REMARK 295 DESCRIBE NON-CRYSTALLOGRAPHIC RELATIONSHIPS AMONG ATOMS
 REMARK 295 IN THIS ENTRY. APPLYING THE APPROPRIATE MTRIX
 REMARK 295 TRANSFORMATION TO THE RESIDUES LISTED FIRST WILL YIELD
 REMARK 295 APPROXIMATE COORDINATES FOR THE RESIDUES LISTED SECOND.
 REMARK 295 CHAIN IDENTIFIERS GIVEN AS "?" REFER TO CHAINS FOR WHICH
 REMARK 295 ATOMS ARE NOT FOUND IN THIS ENTRY.
 REMARK 295
 REMARK 295 APPLIED TO TRANSFORMED TO
 REMARK 295 TRANSFORM CHAIN RESIDUES CHAIN RESIDUES RMSD
 REMARK 295 SSS
 REMARK 295 M 1 B 11 .. 91 A 11 .. 91 1.020
 REMARK 295 M 2 A 11 .. 91 C 11 .. 91 1.677
 REMARK 295 M 3 D 11 .. 91 A 11 .. 91 1.926
 REMARK 295 M 4 C 11 .. 91 B 11 .. 91 0.620
 REMARK 295 M 5 D 11 .. 91 B 11 .. 91 1.764

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FIGURE 8A-5

REMARK 295 M 6 D 11 .. 91 C 11 .. 91 1.810
REMARK 295 M 7 C 11 .. 91 A 11 .. 91 0.898
REMARK 295
REMARK 295 WHERE SSS -> COLUMNS 8-10 OF MTRIX RECORDS
REMARK 295
REMARK 295 REMARK:
REMARK 295 TRANSFORMATION RELATES CHAIN B TO CHAIN A; INCLUDING
REMARK 295 RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN C TO CHAIN A; INCLUDING
REMARK 295 RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN D TO CHAIN A; INCLUDING
REMARK 295 RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN C TO CHAIN B; INCLUDING
REMARK 295 RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN D TO CHAIN B; INCLUDING
REMARK 295 RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN D TO CHAIN C; INCLUDING
REMARK 295 RESIDUES 11-90 AND 104-126.
REMARK 295 TRANSFORMATION RELATES CHAIN CD DIMER TO CHAIN AB DIMER;
REMARK 295 INCLUDING RESIDUES A11-91,A104-126,B11-B90,B104-127,
REMARK 295 C11-91,C104-126,D11-90,D104-127
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470 M RES CSSEQI ATOMS
REMARK 470 ASN A 11 CG OD1 ND2
REMARK 470 VAL A 12 CG1 CG2
REMARK 470 LYS A 13 CG CD CE NZ
REMARK 470 LYS A 91 CG CD CE NZ
REMARK 470 LYS A 127 CG CD CE NZ
REMARK 470 SER A 133 OG
REMARK 470 ASN B 11 CG OD1 ND2
REMARK 470 LYS B 13 CG CD CE NZ
REMARK 470 ASN B 93 CG OD1 ND2
REMARK 470 LYS B 96 CG CD CE NZ
REMARK 470 ASP B 97 CG OD1 OD2
REMARK 470 LYS B 103 CG CD CE NZ
REMARK 470 ASP B 128 CG OD1 OD2
REMARK 470 ASP B 137 CG OD1 OD2
REMARK 470 ASN C 11 CG OD1 ND2
REMARK 470 LYS C 13 CG CD CE NZ
REMARK 470 LEU C 39 CG CD1 CD2
REMARK 470 ASN D 11 CG OD1 ND2
REMARK 470 LYS D 13 CG CD CE NZ
REMARK 470 VAL D 90 CG1 CG2
REMARK 470 GLU D 106 CG CD OE1 OE2
REMARK 470 LYS D 127 CG CD CE NZ
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS
REMARK 500
REMARK 500 THE FOLLOWING ATOMS THAT ARE RELATED BY CRYSTALLOGRAPHIC
REMARK 500 SYMMETRY ARE IN CLOSE CONTACT. AN ATOM LOCATED WITHIN 0.15
REMARK 500 ANGSTROMS OF A SYMMETRY RELATED ATOM IS ASSUMED TO BE ON A
REMARK 500 SPECIAL POSITION AND IS, THEREFORE, LISTED IN REMARK 375
REMARK 500 INSTEAD OF REMARK 500. ATOMS WITH NON-BLANK ALTERNATE
REMARK 500 LOCATION INDICATORS ARE NOT INCLUDED IN THE CALCULATIONS.
REMARK 500

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FIGURE 8A-6

REMARK 500 DISTANCE CUTOFF:
 REMARK 500 2.2 ANGSTROMS FOR CONTACTS NOT INVOLVING HYDROGEN ATOMS
 REMARK 500 1.6 ANGSTROMS FOR CONTACTS INVOLVING HYDROGEN ATOMS
 REMARK 500
 REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI SSYMOP DISTANCE
 REMARK 500 CA CA 1021 O VAL A 139 3655 2.18
 REMARK 500
 REMARK 500 REMARK: NULL
 REMARK 600
 REMARK 600 HETEROGEN
 REMARK 600 1PE: ONLY PART OF THE PEG400 CHAIN IS ORDERED IN THE
 REMARK 600 STRUCTURE.
 REMARK 999
 REMARK 999 SEQUENCE
 REMARK 999 1SCF A SWS P21583 1 - 35 NOT IN ATOMS LIST
 REMARK 999 1SCF A SWS P21583 167 - 273 NOT IN ATOMS LIST
 REMARK 999 1SCF B SWS P21583 1 - 35 NOT IN ATOMS LIST
 REMARK 999 1SCF B SWS P21583 164 - 273 NOT IN ATOMS LIST
 REMARK 999 1SCF C SWS P21583 1 - 35 NOT IN ATOMS LIST
 REMARK 999 1SCF C SWS P21583 152 - 273 NOT IN ATOMS LIST
 REMARK 999 1SCF D SWS P21583 1 - 35 NOT IN ATOMS LIST
 REMARK 999 1SCF D SWS P21583 153 - 273 NOT IN ATOMS LIST
 DBREF 1SCF A 11 91 SWS P21583 SCF_HUMAN 36 116
 DBREF 1SCF A 104 141 SWS P21583 SCF_HUMAN 129 166
 DBREF 1SCF B 11 129 SWS P21583 SCF_HUMAN 36 154
 DBREF 1SCF B 137 138 SWS P21583 SCF_HUMAN 162 163
 DBREF 1SCF C 11 91 SWS P21583 SCF_HUMAN 36 116
 DBREF 1SCF C 104 126 SWS P21583 SCF_HUMAN 129 151
 DBREF 1SCF D 11 90 SWS P21583 SCF_HUMAN 36 115
 DBREF 1SCF D 104 127 SWS P21583 SCF_HUMAN 129 152
 SEQADV 1SCF MSE A 27 SWS P21583 MET 52 MODIFIED
 SEQADV 1SCF MSE A 36 SWS P21583 MET 61 MODIFIED
 SEQADV 1SCF MSE A 48 SWS P21583 MET 73 MODIFIED
 SEQADV 1SCF A SWS P21583 GLU 117 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 ASN 118 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 SER 119 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 SER 120 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 LYS 121 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 ASP 122 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 LEU 123 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 LYS 124 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 LYS 125 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 SER 126 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 PHE 127 GAP IN PDB ENTRY
 SEQADV 1SCF A SWS P21583 LYS 128 GAP IN PDB ENTRY
 SEQADV 1SCF MSE B 27 SWS P21583 MET 52 MODIFIED
 SEQADV 1SCF MSE B 36 SWS P21583 MET 61 MODIFIED
 SEQADV 1SCF MSE B 48 SWS P21583 MET 73 MODIFIED
 SEQADV 1SCF B SWS P21583 VAL 155 GAP IN PDB ENTRY
 SEQADV 1SCF B SWS P21583 VAL 156 GAP IN PDB ENTRY
 SEQADV 1SCF B SWS P21583 ALA 157 GAP IN PDB ENTRY
 SEQADV 1SCF B SWS P21583 SER 158 GAP IN PDB ENTRY
 SEQADV 1SCF B SWS P21583 GLU 159 GAP IN PDB ENTRY
 SEQADV 1SCF B SWS P21583 THR 160 GAP IN PDB ENTRY
 SEQADV 1SCF B SWS P21583 SER 161 GAP IN PDB ENTRY
 SEQADV 1SCF MSE C 27 SWS P21583 MET 52 MODIFIED
 SEQADV 1SCF MSE C 36 SWS P21583 MET 61 MODIFIED
 SEQADV 1SCF MSE C 48 SWS P21583 MET 73 MODIFIED
 SEQADV 1SCF C SWS P21583 GLU 117 GAP IN PDB ENTRY
 SEQADV 1SCF C SWS P21583 ASN 118 GAP IN PDB ENTRY

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FIGURE 8A-7

| | | | | | | | | | | | | | | |
|-------------|-----|-----|--------|-----|--------|-----|-----|----------|-------|-----|-----|-----|-----|-----|
| SEQADV 1SCF | C | SWS | P21583 | SER | 119 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | C | SWS | P21583 | SER | 120 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | C | SWS | P21583 | LYS | 121 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | C | SWS | P21583 | ASP | 122 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | C | SWS | P21583 | LEU | 123 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | C | SWS | P21583 | LYS | 124 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | C | SWS | P21583 | LYS | 125 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | C | SWS | P21583 | SER | 126 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | C | SWS | P21583 | PHE | 127 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | C | SWS | P21583 | LYS | 128 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | MSE | D | 27 | SWS | P21583 | MET | 52 | MODIFIED | | | | | | |
| SEQADV 1SCF | MSE | D | 36 | SWS | P21583 | MET | 61 | MODIFIED | | | | | | |
| SEQADV 1SCF | MSE | D | 48 | SWS | P21583 | MET | 73 | MODIFIED | | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | LYS | 116 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | GLU | 117 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | ASN | 118 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | SER | 119 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | SER | 120 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | LYS | 121 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | ASP | 122 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | LEU | 123 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | LYS | 124 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | LYS | 125 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | SER | 126 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | PHE | 127 | GAP | IN | PDB | ENTRY | | | | | |
| SEQADV 1SCF | D | SWS | P21583 | LYS | 128 | GAP | IN | PDB | ENTRY | | | | | |
| SEQRES 1 A | 273 | MET | LYS | LYS | THR | GLN | THR | TRP | ILE | LEU | THR | CYS | ILE | TYR |
| SEQRES 2 A | 273 | LEU | GLN | LEU | LEU | LEU | PHE | ASN | PRO | LEU | VAL | LYS | THR | GLU |
| SEQRES 3 A | 273 | GLY | ILE | CYS | ARG | ASN | ARG | VAL | THR | ASN | ASN | VAL | LYS | ASP |
| SEQRES 4 A | 273 | VAL | THR | LYS | LEU | VAL | ALA | ASN | LEU | PRO | LYS | ASP | TYR | MSE |
| SEQRES 5 A | 273 | ILE | THR | LEU | LYS | TYR | VAL | PRO | GLY | MSE | ASP | VAL | LEU | PRO |
| SEQRES 6 A | 273 | SER | HIS | CYS | TRP | ILE | SER | GLU | MSE | VAL | VAL | GLN | LEU | SER |
| SEQRES 7 A | 273 | ASP | SER | LEU | THR | ASP | LEU | LEU | ASP | LYS | PHE | SER | ASN | ILE |
| SEQRES 8 A | 273 | SER | GLU | GLY | LEU | SER | ASN | TYR | SER | ILE | ILE | ASP | LYS | LEU |
| SEQRES 9 A | 273 | VAL | ASN | ILE | VAL | ASP | ASP | LEU | VAL | GLU | CYS | VAL | LYS | GLU |
| SEQRES 10 A | 273 | ASN | SER | SER | LYS | ASP | LEU | LYS | LYS | SER | PHE | LYS | SER | PRO |
| SEQRES 11 A | 273 | GLU | PRO | ARG | LEU | PHE | THR | PRO | GLU | GLU | PHE | PHE | ARG | ILE |
| SEQRES 12 A | 273 | PHE | ASN | ARG | SER | ILE | ASP | ALA | PHE | LYS | ASP | PHE | VAL | VAL |
| SEQRES 13 A | 273 | ALA | SER | GLU | THR | SER | ASP | CYS | VAL | VAL | SER | SER | THR | LEU |
| SEQRES 14 A | 273 | SER | PRO | GLU | LYS | ASP | SER | ARG | VAL | SER | VAL | THR | LYS | PRO |
| SEQRES 15 A | 273 | PHE | MET | LEU | PRO | PRO | VAL | ALA | ALA | SER | SER | LEU | ARG | ASN |
| SEQRES 16 A | 273 | ASP | SER | SER | SER | ASN | ARG | LYS | ALA | LYS | ASN | PRO | PRO | |
| SEQRES 17 A | 273 | GLY | ASP | SER | SER | LEU | HIS | TRP | ALA | ALA | MET | ALA | LEU | PRO |
| SEQRES 18 A | 273 | ALA | LEU | PHE | SER | LEU | ILE | ILE | GLY | PHE | ALA | PHE | GLY | ALA |
| SEQRES 19 A | 273 | LEU | TYR | TRP | LYS | LYS | ARG | GLN | PRO | SER | LEU | THR | ARG | ALA |
| SEQRES 20 A | 273 | VAL | GLU | ASN | ILE | GLN | ILE | ASN | GLU | GLU | ASP | ASN | GLU | ILE |
| SEQRES 21 A | 273 | SER | MET | LEU | GLN | GLU | LYS | GLU | ARG | GLU | PHE | GLN | GLU | VAL |
| SEQRES 1 B | 273 | MET | LYS | LYS | THR | GLN | THR | TRP | ILE | LEU | THR | CYS | ILE | TYR |
| SEQRES 2 B | 273 | LEU | GLN | LEU | LEU | LEU | PHE | ASN | PRO | LEU | VAL | LYS | THR | GLU |
| SEQRES 3 B | 273 | GLY | ILE | CYS | ARG | ASN | ARG | VAL | THR | ASN | ASN | VAL | LYS | ASP |
| SEQRES 4 B | 273 | VAL | THR | LYS | LEU | VAL | ALA | ASN | LEU | PRO | LYS | ASP | TYR | MSE |
| SEQRES 5 B | 273 | ILE | THR | LEU | LYS | TYR | VAL | PRO | GLY | MSE | ASP | VAL | LEU | PRO |
| SEQRES 6 B | 273 | SER | HIS | CYS | TRP | ILE | SER | GLU | MSE | VAL | VAL | GLN | LEU | SER |
| SEQRES 7 B | 273 | ASP | SER | LEU | THR | ASP | LEU | LEU | ASP | LYS | PHE | SER | ASN | ILE |
| SEQRES 8 B | 273 | SER | GLU | GLY | LEU | SER | ASN | TYR | SER | ILE | ILE | ASP | LYS | LEU |
| SEQRES 9 B | 273 | VAL | ASN | ILE | VAL | ASP | ASP | LEU | VAL | GLU | CYS | VAL | LYS | GLU |
| SEQRES 10 B | 273 | ASN | SER | SER | LYS | ASP | LEU | LYS | LYS | SER | PHE | LYS | SER | PRO |
| SEQRES 11 B | 273 | GLU | PRO | ARG | LEU | PHE | THR | PRO | GLU | GLU | PHE | PHE | ARG | ILE |
| SEQRES 12 B | 273 | PHE | ASN | ARG | SER | ILE | ASP | ALA | PHE | LYS | ASP | PHE | VAL | VAL |
| SEQRES 13 B | 273 | ALA | SER | GLU | THR | SER | ASP | CYS | VAL | VAL | SER | SER | THR | LEU |

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FIGURE 8A-8

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FIGURE 8A-9

| | | | | | | | | |
|--------|------|-------|---------------------|-------|-------|------------------|-------|------------------------|
| MODRES | 1SCF | MSE | D | 36 | MET | SELENOMETHIONINE | | |
| MODRES | 1SCF | MSE | D | 48 | MET | SELENOMETHIONINE | | |
| HET | MSE | A | 27 | 8 | | | | |
| HET | MSE | A | 36 | 8 | | | | |
| HET | MSE | A | 48 | 8 | | | | |
| HET | MSE | B | 27 | 8 | | | | |
| HET | MSE | B | 36 | 8 | | | | |
| HET | MSE | B | 48 | 8 | | | | |
| HET | MSE | C | 27 | 8 | | | | |
| HET | MSE | C | 36 | 8 | | | | |
| HET | MSE | C | 48 | 8 | | | | |
| HET | MSE | D | 27 | 8 | | | | |
| HET | MSE | D | 36 | 8 | | | | |
| HET | MSE | D | 48 | 8 | | | | |
| HET | CA | | 1021 | 1 | | | | |
| HET | CA | | 1022 | 1 | | | | |
| HET | CA | | 1023 | 1 | | | | |
| HET | 1PE | | 1 | 16 | | | | |
| HETNAM | | MSE | SELENOMETHIONINE | | | | | |
| HETNAM | | CA | CALCIUM ION | | | | | |
| HETNAM | | 1PE | POLYETHYLENE GLYCOL | | | | | |
| HETSYN | | 1PE | PEG400 | | | | | |
| FORMUL | 1 | MSE | 3(C5 H11 N1 O2 SE1) | | | | | |
| FORMUL | 2 | MSE | 3(C5 H11 N1 O2 SE1) | | | | | |
| FORMUL | 3 | MSE | 3(C5 H11 N1 O2 SE1) | | | | | |
| FORMUL | 4 | MSE | 3(C5 H11 N1 O2 SE1) | | | | | |
| FORMUL | 5 | CA | 3(CA1 2+) | | | | | |
| FORMUL | 6 | 1PE | C10 H22 O6 | | | | | |
| FORMUL | 7 | HOH | *264(H2 O1) | | | | | |
| HELIX | 1 | 1 | VAL A | 12 | ASN A | 21 | 1 | 10 |
| HELIX | 2 | 2 | SER A | 41 | CYS A | 43 | 5 | 3 |
| HELIX | 3 | 3 | SER A | 46 | LYS A | 62 | 5 | 17 |
| HELIX | 4 | 4 | ASN A | 72 | CYS A | 89 | 1 | 18 |
| HELIX | 5 | 5 | PRO A | 112 | LYS A | 127 | 1 | 16 |
| HELIX | 6 | 6 | VAL B | 12 | ASN B | 21 | 1 | 10 |
| HELIX | 7 | 7 | SER B | 41 | CYS B | 43 | 5 | 3 |
| HELIX | 8 | 8 | SER B | 46 | LYS B | 62 | 5 | 17 |
| HELIX | 9 | 9 | ASN B | 72 | GLU B | 92 | 1 | 21 |
| HELIX | 10 | 10 | PRO B | 112 | LYS B | 127 | 1 | 16 |
| HELIX | 11 | 11 | VAL C | 12 | ASN C | 21 | 1 | 10 |
| HELIX | 12 | 12 | SER C | 41 | LYS C | 62 | 1 | 22 |
| HELIX | 13 | 13 | ASN C | 72 | VAL C | 90 | 1 | 19 |
| HELIX | 14 | 14 | PRO C | 112 | ASP C | 124 | 1 | 13 |
| HELIX | 15 | 15 | VAL D | 12 | ASN D | 21 | 1 | 10 |
| HELIX | 16 | 16 | SER D | 41 | CYS D | 43 | 5 | 3 |
| HELIX | 17 | 17 | SER D | 46 | LYS D | 62 | 5 | 17 |
| HELIX | 18 | 18 | ASN D | 72 | CYS D | 89 | 1 | 18 |
| HELIX | 19 | 19 | PRO D | 112 | ALA D | 125 | 1 | 14 |
| SHEET | 1 | A 2 | THR A | 29 | LYS A | 31 | 0 | |
| SHEET | 2 | A 2 | PRO A | 107 | LEU A | 109 | -1 | N ARG A 108 O LEU A 30 |
| SHEET | 1 | B 2 | THR B | 29 | LYS B | 31 | 0 | |
| SHEET | 2 | B 2 | PRO B | 107 | LEU B | 109 | -1 | N ARG B 108 O LEU B 30 |
| SHEET | 1 | C 2 | THR C | 29 | LYS C | 31 | 0 | |
| SHEET | 2 | C 2 | PRO C | 107 | LEU C | 109 | -1 | N ARG C 108 O LEU C 30 |
| SHEET | 1 | D 2 | THR D | 29 | LYS D | 31 | 0 | |
| SHEET | 2 | D 2 | PRO D | 107 | LEU D | 109 | -1 | N ARG D 108 O LEU D 30 |
| SSBOND | 1 | CYS A | 43 | CYS A | 138 | | | |
| SSBOND | 2 | CYS B | 43 | CYS B | 138 | | | |
| LINK | | N | MSE A | 27 | | C | TYR A | 26 |
| LINK | | C | MSE A | 27 | | N | ILE A | 28 |

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FIGURE 8A-10

| | | | | | | | | | | | |
|--------|----------|-----------|-----------|-----------|-------|--------|-------|-----------|-------|-------|---|
| LINK | N | MSE | A | 36 | C | GLY | A | 35 | | | |
| LINK | C | MSE | A | 36 | N | ASP | A | 37 | | | |
| LINK | N | MSE | A | 48 | C | GLU | A | 47 | | | |
| LINK | C | MSE | A | 48 | N | VAL | A | 49 | | | |
| LINK | N | MSE | B | 27 | C | TYR | B | 26 | | | |
| LINK | C | MSE | B | 27 | N | ILE | B | 28 | | | |
| LINK | N | MSE | B | 36 | C | GLY | B | 35 | | | |
| LINK | C | MSE | B | 36 | N | ASP | B | 37 | | | |
| LINK | N | MSE | B | 48 | C | GLU | B | 47 | | | |
| LINK | C | MSE | B | 48 | N | VAL | B | 49 | | | |
| LINK | N | MSE | C | 27 | C | TYR | C | 26 | | | |
| LINK | C | MSE | C | 27 | N | ILE | C | 28 | | | |
| LINK | N | MSE | C | 36 | C | GLY | C | 35 | | | |
| LINK | C | MSE | C | 36 | N | ASP | C | 37 | | | |
| LINK | N | MSE | C | 48 | C | GLU | C | 47 | | | |
| LINK | C | MSE | C | 48 | N | VAL | C | 49 | | | |
| LINK | N | MSE | D | 27 | C | TYR | D | 26 | | | |
| LINK | C | MSE | D | 27 | N | ILE | D | 28 | | | |
| LINK | N | MSE | D | 36 | C | GLY | D | 35 | | | |
| LINK | C | MSE | D | 36 | N | ASP | D | 37 | | | |
| LINK | N | MSE | D | 48 | C | GLU | D | 47 | | | |
| LINK | C | MSE | D | 48 | N | VAL | D | 49 | | | |
| LINK | CA | CA | 1021 | | O | HOH | 1024 | | | | |
| LINK | CA | CA | 1021 | | O | HOH | 1025 | | | | |
| LINK | CA | CA | 1023 | | O | HOH | 1027 | | | | |
| LINK | CA | CA | 1023 | | O | HOH | 1028 | | | | |
| LINK | CA | CA | 1023 | | O | HOH | 1029 | | | | |
| CISPEP | 1 | SER | A | 104 | PRO | A | 105 | 0 | -0.10 | | |
| CRYST1 | 71.820 | 82.550 | 88.190 | 90.00 | 90.00 | 90.00 | P | 21 | 21 | 21 | 4 |
| ORIGX1 | 1.000000 | 0.000000 | 0.000000 | | | | | 0.00000 | | | |
| ORIGX2 | 0.000000 | 1.000000 | 0.000000 | | | | | 0.00000 | | | |
| ORIGX3 | 0.000000 | 0.000000 | 1.000000 | | | | | 0.00000 | | | |
| SCALE1 | 0.013924 | 0.000000 | 0.000000 | | | | | 0.00000 | | | |
| SCALE2 | 0.000000 | 0.012114 | 0.000000 | | | | | 0.00000 | | | |
| SCALE3 | 0.000000 | 0.000000 | 0.011339 | | | | | 0.00000 | | | |
| MTRIX1 | 1 | 0.915300 | 0.368400 | 0.162800 | | | | -10.34380 | | 1 | |
| MTRIX2 | 1 | 0.357100 | -0.929200 | 0.095000 | | | | 35.55670 | | 1 | |
| MTRIX3 | 1 | 0.186300 | -0.028800 | -0.982100 | | | | 43.17570 | | 1 | |
| MTRIX1 | 2 | -0.935658 | -0.315827 | -0.157471 | | | | 63.79985 | | 1 | |
| MTRIX2 | 2 | -0.265278 | 0.923709 | -0.276386 | | | | 17.94411 | | 1 | |
| MTRIX3 | 2 | 0.232747 | -0.216829 | -0.948058 | | | | 63.68074 | | 1 | |
| MTRIX1 | 3 | -0.994700 | 0.088300 | -0.051700 | | | | 54.54720 | | 1 | |
| MTRIX2 | 3 | -0.094000 | -0.988400 | 0.119100 | | | | 48.88150 | | 1 | |
| MTRIX3 | 3 | -0.040600 | 0.123400 | 0.991500 | | | | -20.54390 | | 1 | |
| MTRIX1 | 4 | -0.991100 | 0.100500 | -0.087800 | | | | 55.16840 | | 1 | |
| MTRIX2 | 4 | -0.117800 | -0.968000 | 0.221700 | | | | 45.07210 | | 1 | |
| MTRIX3 | 4 | -0.062700 | 0.230100 | 0.971100 | | | | -21.92400 | | 1 | |
| MTRIX1 | 5 | -0.951900 | -0.248300 | 0.179700 | | | | 52.26270 | | 1 | |
| MTRIX2 | 5 | -0.277100 | 0.947600 | -0.158800 | | | | 13.33780 | | 1 | |
| MTRIX3 | 5 | -0.130900 | -0.200900 | -0.970800 | | | | 74.41510 | | 1 | |
| MTRIX1 | 6 | 0.984200 | 0.147100 | -0.098100 | | | | 0.55340 | | 1 | |
| MTRIX2 | 6 | 0.142600 | -0.988400 | -0.052100 | | | | 52.60730 | | 1 | |
| MTRIX3 | 6 | -0.104600 | 0.037300 | -0.993800 | | | | 86.74100 | | 1 | |
| MTRIX1 | 7 | -0.955400 | -0.244200 | 0.166100 | | | | 52.84290 | | 1 | |
| MTRIX2 | 7 | -0.269500 | 0.950900 | -0.152200 | | | | 12.52990 | | 1 | |
| MTRIX3 | 7 | -0.120800 | -0.190100 | -0.974300 | | | | 73.76110 | | 1 | |
| ATOM | 1 | N | ASN | A | 11 | 10.232 | 3.110 | 20.636 | 1.00 | 60.07 | |
| ATOM | 2 | CA | ASN | A | 11 | 9.176 | 3.892 | 19.994 | 1.00 | 59.79 | |
| ATOM | 3 | C | ASN | A | 11 | 9.647 | 5.204 | 19.309 | 1.00 | 59.52 | |
| ATOM | 4 | O | ASN | A | 11 | 9.661 | 6.288 | 19.910 | 1.00 | 59.97 | |

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FIGURE 8A-11

| | | | | | | | | | | |
|------|----|-----|-------|----|--------|--------|--------|------|-------|---|
| ATOM | 5 | CB | ASN A | 11 | 8.113 | 4.228 | 21.038 | 1.00 | 60.46 | C |
| ATOM | 6 | N | VAL A | 12 | 10.013 | 5.143 | 18.009 | 1.00 | 57.40 | N |
| ATOM | 7 | CA | VAL A | 12 | 10.715 | 6.225 | 17.309 | 1.00 | 53.71 | C |
| ATOM | 8 | C | VAL A | 12 | 9.844 | 7.387 | 16.820 | 1.00 | 50.84 | O |
| ATOM | 9 | O | VAL A | 12 | 10.343 | 8.268 | 16.130 | 1.00 | 51.46 | C |
| ATOM | 10 | CB | VAL A | 12 | 11.541 | 5.657 | 16.126 | 1.00 | 53.25 | O |
| ATOM | 11 | N | LYS A | 13 | 8.543 | 7.490 | 17.147 | 1.00 | 49.07 | C |
| ATOM | 12 | CA | LYS A | 13 | 7.721 | 8.640 | 16.756 | 1.00 | 44.35 | N |
| ATOM | 13 | C | LYS A | 13 | 8.114 | 9.879 | 17.542 | 1.00 | 42.88 | C |
| ATOM | 14 | O | LYS A | 13 | 8.271 | 10.995 | 17.007 | 1.00 | 41.79 | O |
| ATOM | 15 | CB | LYS A | 13 | 6.258 | 8.378 | 17.093 | 1.00 | 44.76 | C |
| ATOM | 16 | N | ASP A | 14 | 8.283 | 9.557 | 18.839 | 1.00 | 38.29 | N |
| ATOM | 17 | CA | ASP A | 14 | 8.609 | 10.545 | 19.818 | 1.00 | 35.56 | C |
| ATOM | 18 | C | ASP A | 14 | 10.068 | 10.894 | 19.718 | 1.00 | 32.01 | C |
| ATOM | 19 | O | ASP A | 14 | 10.389 | 12.060 | 19.896 | 1.00 | 30.80 | O |
| ATOM | 20 | CB | ASP A | 14 | 8.151 | 10.072 | 21.200 | 1.00 | 38.77 | C |
| ATOM | 21 | CG | ASP A | 14 | 6.725 | 10.518 | 21.630 | 1.00 | 43.77 | O |
| ATOM | 22 | OD1 | ASP A | 14 | 6.046 | 11.324 | 20.969 | 1.00 | 45.53 | C |
| ATOM | 23 | OD2 | ASP A | 14 | 6.269 | 10.057 | 22.680 | 1.00 | 47.33 | O |
| ATOM | 24 | N | VAL A | 15 | 10.939 | 9.938 | 19.360 | 1.00 | 28.31 | N |
| ATOM | 25 | CA | VAL A | 15 | 12.335 | 10.224 | 19.089 | 1.00 | 27.35 | C |
| ATOM | 26 | C | VAL A | 15 | 12.510 | 11.219 | 17.959 | 1.00 | 29.06 | C |
| ATOM | 27 | O | VAL A | 15 | 13.265 | 12.166 | 18.138 | 1.00 | 32.49 | O |
| ATOM | 28 | CB | VAL A | 15 | 13.191 | 8.976 | 18.792 | 1.00 | 26.33 | C |
| ATOM | 29 | CG1 | VAL A | 15 | 14.623 | 9.347 | 18.405 | 1.00 | 20.32 | O |
| ATOM | 30 | CG2 | VAL A | 15 | 13.215 | 8.064 | 20.008 | 1.00 | 24.37 | C |
| ATOM | 31 | N | THR A | 16 | 11.858 | 11.085 | 16.807 | 1.00 | 28.42 | C |
| ATOM | 32 | CA | THR A | 16 | 11.968 | 12.085 | 15.758 | 1.00 | 27.97 | N |
| ATOM | 33 | C | THR A | 16 | 11.386 | 13.413 | 16.208 | 1.00 | 25.43 | C |
| ATOM | 34 | O | THR A | 16 | 12.020 | 14.418 | 15.905 | 1.00 | 25.82 | O |
| ATOM | 35 | CB | THR A | 16 | 11.357 | 11.646 | 14.385 | 1.00 | 27.70 | C |
| ATOM | 36 | OG1 | THR A | 16 | 9.959 | 11.529 | 14.588 | 1.00 | 32.27 | O |
| ATOM | 37 | CG2 | THR A | 16 | 11.931 | 10.335 | 13.912 | 1.00 | 25.71 | C |
| ATOM | 38 | N | LYS A | 17 | 10.243 | 13.459 | 16.928 | 1.00 | 24.83 | N |
| ATOM | 39 | CA | LYS A | 17 | 9.701 | 14.698 | 17.482 | 1.00 | 23.60 | C |
| ATOM | 40 | C | LYS A | 17 | 10.659 | 15.401 | 18.410 | 1.00 | 21.54 | C |
| ATOM | 41 | O | LYS A | 17 | 10.756 | 16.624 | 18.373 | 1.00 | 23.88 | O |
| ATOM | 42 | CB | LYS A | 17 | 8.365 | 14.488 | 18.206 | 1.00 | 27.08 | C |
| ATOM | 43 | CG | LYS A | 17 | 7.291 | 14.120 | 17.198 | 1.00 | 34.84 | C |
| ATOM | 44 | CD | LYS A | 17 | 5.881 | 14.040 | 17.781 | 1.00 | 40.64 | C |
| ATOM | 45 | CE | LYS A | 17 | 4.800 | 13.911 | 16.665 | 1.00 | 45.98 | C |
| ATOM | 46 | NZ | LYS A | 17 | 4.607 | 12.559 | 16.140 | 1.00 | 48.58 | N |
| ATOM | 47 | N | LEU A | 18 | 11.417 | 14.646 | 19.212 | 1.00 | 19.73 | N |
| ATOM | 48 | CA | LEU A | 18 | 12.377 | 15.207 | 20.151 | 1.00 | 17.98 | C |
| ATOM | 49 | C | LEU A | 18 | 13.544 | 15.778 | 19.401 | 1.00 | 17.55 | C |
| ATOM | 50 | O | LEU A | 18 | 13.813 | 16.959 | 19.523 | 1.00 | 17.68 | O |
| ATOM | 51 | CB | LEU A | 18 | 12.875 | 14.144 | 21.121 | 1.00 | 17.63 | C |
| ATOM | 52 | CG | LEU A | 18 | 13.850 | 14.582 | 22.216 | 1.00 | 15.34 | C |
| ATOM | 53 | CD1 | LEU A | 18 | 13.278 | 15.668 | 23.080 | 1.00 | 15.28 | C |
| ATOM | 54 | CD2 | LEU A | 18 | 14.253 | 13.389 | 23.032 | 1.00 | 14.40 | C |
| ATOM | 55 | N | VAL A | 19 | 14.189 | 14.952 | 18.577 | 1.00 | 18.35 | N |
| ATOM | 56 | CA | VAL A | 19 | 15.187 | 15.421 | 17.628 | 1.00 | 19.40 | C |
| ATOM | 57 | C | VAL A | 19 | 14.757 | 16.628 | 16.824 | 1.00 | 18.97 | C |
| ATOM | 58 | O | VAL A | 19 | 15.533 | 17.562 | 16.711 | 1.00 | 22.36 | O |
| ATOM | 59 | CB | VAL A | 19 | 15.668 | 14.325 | 16.729 | 1.00 | 18.19 | C |
| ATOM | 60 | CG1 | VAL A | 19 | 16.675 | 14.817 | 15.708 | 1.00 | 20.68 | C |
| ATOM | 61 | CG2 | VAL A | 19 | 16.422 | 13.390 | 17.612 | 1.00 | 19.91 | C |
| ATOM | 62 | N | ALA A | 20 | 13.530 | 16.732 | 16.366 | 1.00 | 18.27 | N |
| ATOM | 63 | CA | ALA A | 20 | 13.105 | 17.946 | 15.719 | 1.00 | 17.82 | C |
| ATOM | 64 | C | ALA A | 20 | 12.923 | 19.074 | 16.711 | 1.00 | 18.90 | C |

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FIGURE 8A-12

| | | | | | | | | | | |
|--------|-----|-----|-------|----|--------|--------|--------|------|-------|---|
| ATOM | 65 | O | ALA A | 20 | 12.977 | 20.244 | 16.352 | 1.00 | 20.70 | O |
| ATOM | 66 | CB | ALA A | 20 | 11.777 | 17.661 | 15.059 | 1.00 | 17.70 | C |
| ATOM | 67 | N | ASN A | 21 | 12.677 | 18.787 | 17.979 | 1.00 | 20.04 | N |
| ATOM | 68 | CA | ASN A | 21 | 12.450 | 19.852 | 18.933 | 1.00 | 20.73 | C |
| ATOM | 69 | C | ASN A | 21 | 13.695 | 20.161 | 19.771 | 1.00 | 20.34 | C |
| ATOM | 70 | O | ASN A | 21 | 13.627 | 20.909 | 20.741 | 1.00 | 21.05 | O |
| ATOM | 71 | CB | ASN A | 21 | 11.235 | 19.456 | 19.751 | 1.00 | 20.84 | C |
| ATOM | 72 | CG | ASN A | 21 | 10.409 | 20.664 | 20.103 | 1.00 | 21.87 | C |
| ATOM | 73 | OD1 | ASN A | 21 | 10.157 | 21.501 | 19.250 | 1.00 | 20.51 | O |
| ATOM | 74 | ND2 | ASN A | 21 | 9.983 | 20.853 | 21.359 | 1.00 | 25.03 | N |
| ATOM | 75 | N | LEU A | 22 | 14.851 | 19.615 | 19.399 | 1.00 | 18.22 | N |
| ATOM | 76 | CA | LEU A | 22 | 16.129 | 19.924 | 20.000 | 1.00 | 17.27 | C |
| ATOM | 77 | C | LEU A | 22 | 17.023 | 20.733 | 19.051 | 1.00 | 19.37 | C |
| ATOM | 78 | O | LEU A | 22 | 17.001 | 20.468 | 17.851 | 1.00 | 19.69 | O |
| ATOM | 79 | CB | LEU A | 22 | 16.856 | 18.631 | 20.432 | 1.00 | 16.17 | C |
| ATOM | 80 | CG | LEU A | 22 | 16.342 | 17.790 | 21.598 | 1.00 | 14.77 | C |
| ATOM | 81 | CD1 | LEU A | 22 | 17.058 | 16.447 | 21.768 | 1.00 | 14.07 | C |
| ATOM | 82 | CD2 | LEU A | 22 | 16.463 | 18.606 | 22.862 | 1.00 | 11.82 | C |
| ATOM | 83 | N | PRO A | 23 | 17.833 | 21.728 | 19.457 | 1.00 | 19.42 | N |
| ATOM | 84 | CA | PRO A | 23 | 18.655 | 22.511 | 18.537 | 1.00 | 19.17 | C |
| ATOM | 85 | C | PRO A | 23 | 19.694 | 21.621 | 17.878 | 1.00 | 20.53 | C |
| ATOM | 86 | O | PRO A | 23 | 20.318 | 20.832 | 18.575 | 1.00 | 21.23 | O |
| ATOM | 87 | CB | PRO A | 23 | 19.341 | 23.488 | 19.459 | 1.00 | 18.21 | C |
| ATOM | 88 | CG | PRO A | 23 | 18.549 | 23.480 | 20.755 | 1.00 | 16.10 | C |
| ATOM | 89 | CD | PRO A | 23 | 18.206 | 22.015 | 20.846 | 1.00 | 17.73 | C |
| ATOM | 90 | N | LYS A | 24 | 19.959 | 21.716 | 16.571 | 1.00 | 23.65 | N |
| ATOM | 91 | CA | LYS A | 24 | 20.937 | 20.852 | 15.866 | 1.00 | 27.23 | C |
| ATOM | 92 | C | LYS A | 24 | 22.388 | 20.847 | 16.370 | 1.00 | 25.36 | C |
| ATOM | 93 | O | LYS A | 24 | 23.179 | 19.918 | 16.149 | 1.00 | 25.16 | O |
| ATOM | 94 | CB | LYS A | 24 | 20.931 | 21.150 | 14.332 | 1.00 | 29.02 | C |
| ATOM | 95 | CG | LYS A | 24 | 19.550 | 20.939 | 13.680 | 1.00 | 36.19 | C |
| ATOM | 96 | CD | LYS A | 24 | 19.557 | 21.512 | 12.245 | 1.00 | 43.22 | C |
| ATOM | 97 | CE | LYS A | 24 | 18.207 | 21.800 | 11.585 | 1.00 | 42.88 | C |
| ATOM | 98 | NZ | LYS A | 24 | 18.433 | 22.694 | 10.448 | 1.00 | 48.02 | N |
| ATOM | 99 | N | ASP A | 25 | 22.712 | 21.900 | 17.110 | 1.00 | 26.32 | N |
| ATOM | 100 | CA | ASP A | 25 | 24.060 | 22.087 | 17.653 | 1.00 | 28.70 | C |
| ATOM | 101 | C | ASP A | 25 | 24.209 | 22.024 | 19.180 | 1.00 | 26.91 | C |
| ATOM | 102 | O | ASP A | 25 | 25.225 | 22.386 | 19.785 | 1.00 | 27.43 | O |
| ATOM | 103 | CB | ASP A | 25 | 24.551 | 23.433 | 17.144 | 1.00 | 30.59 | C |
| ATOM | 104 | CG | ASP A | 25 | 23.780 | 24.615 | 17.684 | 1.00 | 33.09 | C |
| ATOM | 105 | OD1 | ASP A | 25 | 22.556 | 24.529 | 17.847 | 1.00 | 34.74 | O |
| ATOM | 106 | OD2 | ASP A | 25 | 24.421 | 25.638 | 17.933 | 1.00 | 37.53 | O |
| ATOM | 107 | N | TYR A | 26 | 23.122 | 21.605 | 19.808 | 1.00 | 24.09 | N |
| ATOM | 108 | CA | TYR A | 26 | 23.165 | 21.289 | 21.189 | 1.00 | 20.96 | C |
| ATOM | 109 | C | TYR A | 26 | 23.821 | 19.937 | 21.246 | 1.00 | 20.04 | C |
| ATOM | 110 | O | TYR A | 26 | 23.282 | 18.951 | 20.780 | 1.00 | 22.61 | O |
| ATOM | 111 | CB | TYR A | 26 | 21.759 | 21.239 | 21.710 | 1.00 | 20.00 | C |
| ATOM | 112 | CG | TYR A | 26 | 21.728 | 20.927 | 23.199 | 1.00 | 23.05 | C |
| ATOM | 113 | CD1 | TYR A | 26 | 22.430 | 21.764 | 24.039 | 1.00 | 20.56 | C |
| ATOM | 114 | CD2 | TYR A | 26 | 21.015 | 19.843 | 23.683 | 1.00 | 22.87 | C |
| ATOM | 115 | CE1 | TYR A | 26 | 22.421 | 21.541 | 25.376 | 1.00 | 23.76 | C |
| ATOM | 116 | CE2 | TYR A | 26 | 20.993 | 19.629 | 25.047 | 1.00 | 22.41 | C |
| ATOM | 117 | CZ | TYR A | 26 | 21.693 | 20.493 | 25.877 | 1.00 | 23.68 | C |
| ATOM | 118 | OH | TYR A | 26 | 21.661 | 20.353 | 27.259 | 1.00 | 22.67 | O |
| HETATM | 119 | N | MSE A | 27 | 25.003 | 19.890 | 21.809 | 1.00 | 21.07 | N |
| HETATM | 120 | CA | MSE A | 27 | 25.716 | 18.643 | 22.008 | 1.00 | 21.95 | C |
| HETATM | 121 | C | MSE A | 27 | 25.325 | 17.906 | 23.296 | 1.00 | 23.63 | C |
| HETATM | 122 | O | MSE A | 27 | 25.089 | 18.481 | 24.371 | 1.00 | 22.77 | O |
| HETATM | 123 | CB | MSE A | 27 | 27.201 | 18.955 | 22.055 | 1.00 | 27.32 | C |
| HETATM | 124 | CG | MSE A | 27 | 27.695 | 19.788 | 20.866 | 1.00 | 28.96 | C |

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FIGURE 8A-13

| | | | | | | | | | | | |
|--------|-----|-----|-----|---|----|--------|--------|--------|------|-------|----|
| HETATM | 125 | SE | MSE | A | 27 | 27.207 | 18.877 | 19.234 | 1.00 | 37.24 | SE |
| HETATM | 126 | CE | MSE | A | 27 | 28.489 | 17.511 | 19.371 | 1.00 | 26.83 | C |
| ATOM | 127 | N | ILE | A | 28 | 25.250 | 16.576 | 23.165 | 1.00 | 26.83 | N |
| ATOM | 128 | CA | ILE | A | 28 | 24.860 | 15.666 | 24.240 | 1.00 | 22.91 | C |
| ATOM | 129 | C | ILE | A | 28 | 26.030 | 14.713 | 24.494 | 1.00 | 21.29 | C |
| ATOM | 130 | O | ILE | A | 28 | 26.530 | 14.075 | 23.571 | 1.00 | 21.02 | C |
| ATOM | 131 | CB | ILE | A | 28 | 23.550 | 14.901 | 23.870 | 1.00 | 20.97 | O |
| ATOM | 132 | CG1 | ILE | A | 28 | 22.372 | 15.818 | 23.534 | 1.00 | 19.78 | C |
| ATOM | 133 | CG2 | ILE | A | 28 | 23.147 | 14.006 | 25.006 | 1.00 | 18.93 | C |
| ATOM | 134 | CD1 | ILE | A | 28 | 21.207 | 15.120 | 22.805 | 1.00 | 16.08 | C |
| ATOM | 135 | N | THR | A | 29 | 26.492 | 14.597 | 25.744 | 1.00 | 20.17 | C |
| ATOM | 136 | CA | THR | A | 29 | 27.592 | 13.727 | 26.087 | 1.00 | 20.16 | N |
| ATOM | 137 | C | THR | A | 29 | 27.065 | 12.315 | 26.319 | 1.00 | 20.21 | C |
| ATOM | 138 | O | THR | A | 29 | 26.051 | 12.081 | 26.988 | 1.00 | 19.29 | C |
| ATOM | 139 | CB | THR | A | 29 | 28.269 | 14.295 | 27.333 | 1.00 | 21.22 | C |
| ATOM | 140 | OG1 | THR | A | 29 | 28.515 | 15.655 | 27.048 | 1.00 | 24.08 | C |
| ATOM | 141 | CG2 | THR | A | 29 | 29.593 | 13.644 | 27.634 | 1.00 | 23.19 | C |
| ATOM | 142 | N | LEU | A | 30 | 27.767 | 11.369 | 25.708 | 1.00 | 18.56 | C |
| ATOM | 143 | CA | LEU | A | 30 | 27.462 | 9.976 | 25.862 | 1.00 | 17.76 | C |
| ATOM | 144 | C | LEU | A | 30 | 28.824 | 9.351 | 25.959 | 1.00 | 18.41 | C |
| ATOM | 145 | O | LEU | A | 30 | 29.738 | 9.774 | 25.283 | 1.00 | 20.72 | C |
| ATOM | 146 | CB | LEU | A | 30 | 26.649 | 9.396 | 24.642 | 1.00 | 19.78 | C |
| ATOM | 147 | CG | LEU | A | 30 | 26.350 | 7.884 | 24.473 | 1.00 | 14.53 | C |
| ATOM | 148 | CD1 | LEU | A | 30 | 25.475 | 7.478 | 25.601 | 1.00 | 18.04 | C |
| ATOM | 149 | CD2 | LEU | A | 30 | 25.629 | 7.525 | 23.205 | 1.00 | 14.92 | C |
| ATOM | 150 | N | LYS | A | 31 | 28.984 | 8.378 | 26.833 | 1.00 | 18.64 | C |
| ATOM | 151 | CA | LYS | A | 31 | 30.176 | 7.575 | 26.918 | 1.00 | 20.71 | C |
| ATOM | 152 | C | LYS | A | 31 | 29.940 | 6.417 | 25.999 | 1.00 | 21.51 | C |
| ATOM | 153 | O | LYS | A | 31 | 28.966 | 5.701 | 26.170 | 1.00 | 23.02 | C |
| ATOM | 154 | CB | LYS | A | 31 | 30.411 | 7.009 | 28.295 | 1.00 | 19.63 | O |
| ATOM | 155 | CG | LYS | A | 31 | 30.788 | 8.066 | 29.309 | 1.00 | 25.85 | C |
| ATOM | 156 | CD | LYS | A | 31 | 31.154 | 7.355 | 30.605 | 1.00 | 29.83 | C |
| ATOM | 157 | CE | LYS | A | 31 | 31.652 | 8.305 | 31.675 | 1.00 | 32.89 | C |
| ATOM | 158 | NZ | LYS | A | 31 | 32.116 | 7.506 | 32.799 | 1.00 | 39.63 | C |
| ATOM | 159 | N | TYR | A | 32 | 30.845 | 6.219 | 25.034 | 1.00 | 24.83 | N |
| ATOM | 160 | CA | TYR | A | 32 | 30.565 | 5.424 | 23.844 | 1.00 | 22.31 | N |
| ATOM | 161 | C | TYR | A | 32 | 31.607 | 4.359 | 23.767 | 1.00 | 19.55 | C |
| ATOM | 162 | O | TYR | A | 32 | 32.759 | 4.667 | 23.946 | 1.00 | 22.18 | C |
| ATOM | 163 | CB | TYR | A | 32 | 30.569 | 6.367 | 22.640 | 1.00 | 25.12 | O |
| ATOM | 164 | CG | TYR | A | 32 | 30.557 | 5.725 | 21.262 | 1.00 | 27.46 | C |
| ATOM | 165 | CD1 | TYR | A | 32 | 31.790 | 5.449 | 20.689 | 1.00 | 26.41 | C |
| ATOM | 166 | CD2 | TYR | A | 32 | 29.369 | 5.437 | 20.613 | 1.00 | 26.10 | C |
| ATOM | 167 | CE1 | TYR | A | 32 | 31.871 | 4.860 | 19.452 | 1.00 | 27.56 | C |
| ATOM | 168 | CE2 | TYR | A | 32 | 29.462 | 4.854 | 19.356 | 1.00 | 29.60 | C |
| ATOM | 169 | CZ | TYR | A | 32 | 30.710 | 4.589 | 18.787 | 1.00 | 28.41 | C |
| ATOM | 170 | OH | TYR | A | 32 | 30.844 | 4.087 | 17.501 | 1.00 | 32.61 | C |
| ATOM | 171 | N | VAL | A | 33 | 31.217 | 3.108 | 23.604 | 1.00 | 20.21 | O |
| ATOM | 172 | CA | VAL | A | 33 | 32.138 | 2.022 | 23.453 | 1.00 | 22.23 | N |
| ATOM | 173 | C | VAL | A | 33 | 32.829 | 2.212 | 22.110 | 1.00 | 24.20 | C |
| ATOM | 174 | O | VAL | A | 33 | 32.156 | 2.231 | 21.078 | 1.00 | 24.76 | O |
| ATOM | 175 | CB | VAL | A | 33 | 31.400 | 0.676 | 23.549 | 1.00 | 23.11 | C |
| ATOM | 176 | CG1 | VAL | A | 33 | 32.297 | -0.537 | 23.309 | 1.00 | 22.36 | O |
| ATOM | 177 | CG2 | VAL | A | 33 | 30.857 | 0.535 | 24.951 | 1.00 | 25.26 | C |
| ATOM | 178 | N | PRO | A | 34 | 34.158 | 2.380 | 22.078 | 1.00 | 25.19 | C |
| ATOM | 179 | CA | PRO | A | 34 | 34.921 | 2.477 | 20.834 | 1.00 | 27.43 | N |
| ATOM | 180 | C | PRO | A | 34 | 34.727 | 1.263 | 19.907 | 1.00 | 27.77 | C |
| ATOM | 181 | O | PRO | A | 34 | 34.907 | 0.101 | 20.291 | 1.00 | 27.65 | C |
| ATOM | 182 | CB | PRO | A | 34 | 36.381 | 2.586 | 21.335 | 1.00 | 29.54 | O |
| ATOM | 183 | CG | PRO | A | 34 | 36.224 | 3.056 | 22.773 | 1.00 | 26.93 | C |
| ATOM | 184 | CD | PRO | A | 34 | 35.043 | 2.269 | 23.245 | 1.00 | 23.54 | C |

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FIGURE 8A-14

| | | | | | | | | | | | |
|--------|-----|-----|-----|---|----|--------|---------|--------|------|-------|----|
| ATOM | 185 | N | GLY | A | 35 | 34.312 | 1.550 | 18.666 | 1.00 | 28.92 | N |
| ATOM | 186 | CA | GLY | A | 35 | 34.175 | 0.517 | 17.650 | 1.00 | 28.59 | C |
| ATOM | 187 | C | GLY | A | 35 | 32.886 | -0.277 | 17.715 | 1.00 | 28.76 | C |
| ATOM | 188 | O | GLY | A | 35 | 32.743 | -1.224 | 16.957 | 1.00 | 29.41 | O |
| HETATM | 189 | N | MSE | A | 36 | 31.923 | 0.064 | 18.569 | 1.00 | 27.95 | N |
| HETATM | 190 | CA | MSE | A | 36 | 30.612 | -0.561 | 18.587 | 1.00 | 28.65 | C |
| HETATM | 191 | C | MSE | A | 36 | 29.809 | -0.477 | 17.276 | 1.00 | 28.45 | C |
| HETATM | 192 | O | MSE | A | 36 | 28.824 | -1.189 | 17.098 | 1.00 | 26.26 | O |
| HETATM | 193 | CB | MSE | A | 36 | 29.774 | 0.036 | 19.739 | 1.00 | 32.71 | C |
| HETATM | 194 | CG | MSE | A | 36 | 29.232 | 1.427 | 19.485 | 1.00 | 34.05 | C |
| HETATM | 195 | SE | MSE | A | 36 | 27.946 | 2.252 | 20.676 | 1.00 | 36.59 | SE |
| HETATM | 196 | CE | MSE | A | 36 | 26.309 | 1.728 | 19.841 | 1.00 | 26.94 | C |
| ATOM | 197 | N | ASP | A | 37 | 30.212 | 0.393 | 16.338 | 1.00 | 30.42 | N |
| ATOM | 198 | CA | ASP | A | 37 | 29.736 | 0.418 | 14.935 | 1.00 | 30.74 | C |
| ATOM | 199 | C | ASP | A | 37 | 30.051 | -0.794 | 14.038 | 1.00 | 27.32 | C |
| ATOM | 200 | O | ASP | A | 37 | 29.344 | -1.054 | 13.064 | 1.00 | 28.97 | O |
| ATOM | 201 | CB | ASP | A | 37 | 30.200 | 1.716 | 14.234 | 1.00 | 33.15 | O |
| ATOM | 202 | CG | ASP | A | 37 | 31.706 | 1.960 | 14.294 | 1.00 | 35.22 | C |
| ATOM | 203 | OD1 | ASP | A | 37 | 32.230 | 2.247 | 15.374 | 1.00 | 42.04 | C |
| ATOM | 204 | OD2 | ASP | A | 37 | 32.369 | 1.875 | 13.275 | 1.00 | 34.84 | O |
| ATOM | 205 | N | VAL | A | 38 | 31.054 | -1.584 | 14.381 | 1.00 | 23.11 | O |
| ATOM | 206 | CA | VAL | A | 38 | 31.471 | -2.713 | 13.566 | 1.00 | 23.69 | N |
| ATOM | 207 | C | VAL | A | 38 | 31.568 | -4.045 | 14.389 | 1.00 | 26.12 | C |
| ATOM | 208 | O | VAL | A | 38 | 31.649 | -5.172 | 13.882 | 1.00 | 27.25 | O |
| ATOM | 209 | CB | VAL | A | 38 | 32.741 | -2.089 | 12.936 | 1.00 | 19.85 | C |
| ATOM | 210 | CG1 | VAL | A | 38 | 34.023 | -2.366 | 13.647 | 1.00 | 16.55 | C |
| ATOM | 211 | CG2 | VAL | A | 38 | 32.825 | -2.379 | 11.512 | 1.00 | 19.54 | C |
| ATOM | 212 | N | LEU | A | 39 | 31.464 | -3.968 | 15.728 | 1.00 | 26.26 | N |
| ATOM | 213 | CA | LEU | A | 39 | 31.505 | -5.113 | 16.640 | 1.00 | 26.07 | C |
| ATOM | 214 | C | LEU | A | 39 | 30.149 | -5.788 | 16.888 | 1.00 | 25.48 | C |
| ATOM | 215 | O | LEU | A | 39 | 29.130 | -5.109 | 16.842 | 1.00 | 23.47 | O |
| ATOM | 216 | CB | LEU | A | 39 | 32.061 | -4.671 | 18.014 | 1.00 | 25.49 | O |
| ATOM | 217 | CG | LEU | A | 39 | 33.515 | -4.307 | 18.156 | 1.00 | 27.97 | C |
| ATOM | 218 | CD1 | LEU | A | 39 | 33.729 | -3.645 | 19.510 | 1.00 | 30.79 | C |
| ATOM | 219 | CD2 | LEU | A | 39 | 34.399 | -5.522 | 17.940 | 1.00 | 23.69 | C |
| ATOM | 220 | N | PRO | A | 40 | 30.017 | -7.086 | 17.192 | 1.00 | 25.65 | N |
| ATOM | 221 | CA | PRO | A | 40 | 28.734 | -7.665 | 17.563 | 1.00 | 27.77 | C |
| ATOM | 222 | C | PRO | A | 40 | 28.061 | -7.004 | 18.792 | 1.00 | 27.59 | C |
| ATOM | 223 | O | PRO | A | 40 | 28.710 | -6.411 | 19.658 | 1.00 | 26.55 | O |
| ATOM | 224 | CB | PRO | A | 40 | 29.102 | -9.122 | 17.683 | 1.00 | 27.41 | O |
| ATOM | 225 | CG | PRO | A | 40 | 30.584 | -9.150 | 18.015 | 1.00 | 26.93 | O |
| ATOM | 226 | CD | PRO | A | 40 | 31.076 | -8.082 | 17.099 | 1.00 | 26.35 | C |
| ATOM | 227 | N | SER | A | 41 | 26.724 | -7.026 | 18.830 | 1.00 | 27.40 | N |
| ATOM | 228 | CA | SER | A | 41 | 26.003 | -6.235 | 19.806 | 1.00 | 26.79 | C |
| ATOM | 229 | C | SER | A | 41 | 26.288 | -6.707 | 21.202 | 1.00 | 27.70 | C |
| ATOM | 230 | O | SER | A | 41 | 26.451 | -5.903 | 22.097 | 1.00 | 29.20 | O |
| ATOM | 231 | CB | SER | A | 41 | 24.540 | -6.240 | 19.558 | 1.00 | 23.46 | C |
| ATOM | 232 | OG | SER | A | 41 | 24.074 | -7.559 | 19.691 | 1.00 | 25.42 | O |
| ATOM | 233 | N | HIS | A | 42 | 26.526 | -8.007 | 21.355 | 1.00 | 29.95 | N |
| ATOM | 234 | CA | HIS | A | 42 | 26.853 | -8.594 | 22.636 | 1.00 | 30.32 | C |
| ATOM | 235 | C | HIS | A | 42 | 28.076 | -7.971 | 23.312 | 1.00 | 29.42 | C |
| ATOM | 236 | O | HIS | A | 42 | 28.270 | -8.138 | 24.524 | 1.00 | 28.56 | O |
| ATOM | 237 | CB | HIS | A | 42 | 27.008 | -10.109 | 22.451 | 1.00 | 35.10 | C |
| ATOM | 238 | CG | HIS | A | 42 | 28.387 | -10.616 | 21.997 | 1.00 | 39.36 | C |
| ATOM | 239 | ND1 | HIS | A | 42 | 29.424 | -10.993 | 22.752 | 1.00 | 43.05 | N |
| ATOM | 240 | CD2 | HIS | A | 42 | 28.829 | -10.644 | 20.694 | 1.00 | 42.30 | C |
| ATOM | 241 | CE1 | HIS | A | 42 | 30.472 | -11.198 | 21.971 | 1.00 | 42.05 | C |
| ATOM | 242 | NE2 | HIS | A | 42 | 30.103 | -10.969 | 20.735 | 1.00 | 41.31 | C |
| ATOM | 243 | N | CYS | A | 43 | 28.888 | -7.246 | 22.533 | 1.00 | 26.69 | N |
| ATOM | 244 | CA | CYS | A | 43 | 30.112 | -6.657 | 23.037 | 1.00 | 29.55 | N |

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FIGURE 8A-17

| | | | | | | | | | | |
|------|-----|-----|-------|----|--------|--------|--------|------|-------|----|
| ATOM | 365 | CG | ASP A | 58 | 23.101 | 15.151 | 32.595 | 1.00 | 41.66 | C |
| ATOM | 366 | OD1 | ASP A | 58 | 23.500 | 15.636 | 33.666 | 1.00 | 45.37 | CO |
| ATOM | 367 | OD2 | ASP A | 58 | 23.204 | 15.764 | 31.502 | 1.00 | 43.30 | N |
| ATOM | 368 | N | LEU A | 59 | 19.762 | 14.614 | 30.994 | 1.00 | 21.38 | C |
| ATOM | 369 | CA | LEU A | 59 | 19.106 | 15.568 | 30.124 | 1.00 | 19.63 | O |
| ATOM | 370 | C | LEU A | 59 | 17.857 | 16.179 | 30.719 | 1.00 | 20.35 | C |
| ATOM | 371 | O | LEU A | 59 | 17.522 | 17.321 | 30.413 | 1.00 | 19.57 | C |
| ATOM | 372 | CB | LEU A | 59 | 18.751 | 14.826 | 28.859 | 1.00 | 19.31 | C |
| ATOM | 373 | CG | LEU A | 59 | 19.006 | 15.498 | 27.551 | 1.00 | 18.41 | N |
| ATOM | 374 | CD1 | LEU A | 59 | 20.161 | 16.496 | 27.615 | 1.00 | 16.32 | C |
| ATOM | 375 | CD2 | LEU A | 59 | 19.225 | 14.401 | 26.555 | 1.00 | 17.59 | C |
| ATOM | 376 | N | LEU A | 60 | 17.163 | 15.410 | 31.587 | 1.00 | 21.63 | C |
| ATOM | 377 | CA | LEU A | 60 | 15.930 | 15.857 | 32.216 | 1.00 | 20.55 | C |
| ATOM | 378 | C | LEU A | 60 | 16.133 | 17.147 | 32.974 | 1.00 | 22.32 | C |
| ATOM | 379 | O | LEU A | 60 | 15.264 | 18.016 | 32.929 | 1.00 | 23.28 | C |
| ATOM | 380 | CB | LEU A | 60 | 15.389 | 14.796 | 33.145 | 1.00 | 17.67 | C |
| ATOM | 381 | CG | LEU A | 60 | 14.680 | 13.601 | 32.538 | 1.00 | 14.57 | C |
| ATOM | 382 | CD1 | LEU A | 60 | 14.293 | 12.641 | 33.643 | 1.00 | 12.83 | C |
| ATOM | 383 | CD2 | LEU A | 60 | 13.462 | 14.048 | 31.847 | 1.00 | 8.22 | C |
| ATOM | 384 | N | ASP A | 61 | 17.338 | 17.285 | 33.558 | 1.00 | 22.42 | N |
| ATOM | 385 | CA | ASP A | 61 | 17.805 | 18.483 | 34.247 | 1.00 | 22.10 | C |
| ATOM | 386 | C | ASP A | 61 | 17.810 | 19.768 | 33.433 | 1.00 | 20.08 | C |
| ATOM | 387 | O | ASP A | 61 | 17.841 | 20.870 | 33.974 | 1.00 | 20.02 | C |
| ATOM | 388 | CB | ASP A | 61 | 19.203 | 18.169 | 34.753 | 1.00 | 28.60 | C |
| ATOM | 389 | CG | ASP A | 61 | 19.803 | 19.159 | 35.750 | 1.00 | 34.29 | C |
| ATOM | 390 | OD1 | ASP A | 61 | 19.459 | 19.073 | 36.931 | 1.00 | 40.97 | O |
| ATOM | 391 | OD2 | ASP A | 61 | 20.616 | 20.006 | 35.356 | 1.00 | 37.85 | O |
| ATOM | 392 | N | LYS A | 62 | 17.721 | 19.693 | 32.105 | 1.00 | 19.76 | O |
| ATOM | 393 | CA | LYS A | 62 | 17.839 | 20.862 | 31.245 | 1.00 | 16.53 | N |
| ATOM | 394 | C | LYS A | 62 | 16.485 | 21.335 | 30.770 | 1.00 | 16.75 | C |
| ATOM | 395 | O | LYS A | 62 | 16.388 | 22.383 | 30.130 | 1.00 | 17.62 | C |
| ATOM | 396 | CB | LYS A | 62 | 18.684 | 20.529 | 30.020 | 1.00 | 18.65 | C |
| ATOM | 397 | CG | LYS A | 62 | 19.986 | 19.755 | 30.233 | 1.00 | 16.80 | C |
| ATOM | 398 | CD | LYS A | 62 | 20.808 | 20.483 | 31.276 | 1.00 | 18.07 | C |
| ATOM | 399 | CE | LYS A | 62 | 22.135 | 19.776 | 31.535 | 1.00 | 23.34 | C |
| ATOM | 400 | NZ | LYS A | 62 | 22.088 | 18.331 | 31.330 | 1.00 | 28.06 | C |
| ATOM | 401 | N | PHE A | 63 | 15.400 | 20.605 | 31.068 | 1.00 | 16.40 | N |
| ATOM | 402 | CA | PHE A | 63 | 14.086 | 20.979 | 30.586 | 1.00 | 16.93 | C |
| ATOM | 403 | C | PHE A | 63 | 13.110 | 21.140 | 31.730 | 1.00 | 17.40 | C |
| ATOM | 404 | O | PHE A | 63 | 13.294 | 20.626 | 32.826 | 1.00 | 17.50 | C |
| ATOM | 405 | CB | PHE A | 63 | 13.576 | 19.942 | 29.574 | 1.00 | 15.08 | C |
| ATOM | 406 | CG | PHE A | 63 | 14.424 | 19.850 | 28.325 | 1.00 | 13.39 | C |
| ATOM | 407 | CD1 | PHE A | 63 | 14.261 | 20.767 | 27.317 | 1.00 | 13.60 | C |
| ATOM | 408 | CD2 | PHE A | 63 | 15.410 | 18.888 | 28.252 | 1.00 | 14.95 | C |
| ATOM | 409 | CE1 | PHE A | 63 | 15.126 | 20.740 | 26.266 | 1.00 | 10.99 | C |
| ATOM | 410 | CE2 | PHE A | 63 | 16.305 | 18.889 | 27.207 | 1.00 | 14.45 | C |
| ATOM | 411 | CZ | PHE A | 63 | 16.150 | 19.832 | 26.229 | 1.00 | 10.95 | C |
| ATOM | 412 | N | SER A | 64 | 12.031 | 21.843 | 31.444 | 1.00 | 19.14 | N |
| ATOM | 413 | CA | SER A | 64 | 10.993 | 22.080 | 32.407 | 1.00 | 21.71 | C |
| ATOM | 414 | C | SER A | 64 | 9.832 | 21.125 | 32.198 | 1.00 | 22.87 | C |
| ATOM | 415 | O | SER A | 64 | 9.431 | 20.758 | 31.098 | 1.00 | 24.09 | C |
| ATOM | 416 | CB | SER A | 64 | 10.533 | 23.508 | 32.261 | 1.00 | 22.47 | C |
| ATOM | 417 | OG | SER A | 64 | 9.408 | 23.881 | 33.049 | 1.00 | 29.46 | C |
| ATOM | 418 | N | ASN A | 65 | 9.298 | 20.809 | 33.363 | 1.00 | 23.97 | N |
| ATOM | 419 | CA | ASN A | 65 | 8.233 | 19.855 | 33.608 | 1.00 | 29.13 | C |
| ATOM | 420 | C | ASN A | 65 | 6.899 | 20.530 | 33.390 | 1.00 | 31.34 | C |
| ATOM | 421 | O | ASN A | 65 | 5.883 | 19.858 | 33.203 | 1.00 | 35.27 | C |
| ATOM | 422 | CB | ASN A | 65 | 8.309 | 19.551 | 35.119 | 1.00 | 30.43 | C |
| ATOM | 423 | CG | ASN A | 65 | 8.097 | 18.117 | 35.514 | 1.00 | 33.16 | C |
| ATOM | 424 | OD1 | ASN A | 65 | 7.488 | 17.258 | 34.873 | 1.00 | 41.60 | C |

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FIGURE 8A-18

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 425 | ND2 | ASN | A | 65 | 8.641 | 17.823 | 36.656 | 1.00 | 34.77 | N |
| ATOM | 426 | N | ILE | A | 66 | 6.892 | 21.862 | 33.561 | 1.00 | 32.62 | N |
| ATOM | 427 | CA | ILE | A | 66 | 5.708 | 22.691 | 33.384 | 1.00 | 33.83 | C |
| ATOM | 428 | C | ILE | A | 66 | 5.681 | 23.071 | 31.918 | 1.00 | 35.58 | C |
| ATOM | 429 | O | ILE | A | 66 | 6.450 | 23.910 | 31.431 | 1.00 | 36.08 | O |
| ATOM | 430 | CB | ILE | A | 66 | 5.752 | 24.000 | 34.223 | 1.00 | 33.21 | C |
| ATOM | 431 | CG1 | ILE | A | 66 | 6.162 | 23.831 | 35.672 | 1.00 | 33.50 | C |
| ATOM | 432 | CG2 | ILE | A | 66 | 4.416 | 24.708 | 34.158 | 1.00 | 31.21 | C |
| ATOM | 433 | CD1 | ILE | A | 66 | 5.330 | 22.784 | 36.415 | 1.00 | 32.37 | C |
| ATOM | 434 | N | SER | A | 67 | 4.782 | 22.424 | 31.201 | 1.00 | 37.23 | C |
| ATOM | 435 | CA | SER | A | 67 | 4.669 | 22.650 | 29.771 | 1.00 | 40.50 | C |
| ATOM | 436 | C | SER | A | 67 | 3.358 | 22.008 | 29.327 | 1.00 | 42.07 | C |
| ATOM | 437 | O | SER | A | 67 | 3.073 | 20.841 | 29.622 | 1.00 | 43.86 | O |
| ATOM | 438 | CB | SER | A | 67 | 5.892 | 21.985 | 29.075 | 1.00 | 40.62 | O |
| ATOM | 439 | OG | SER | A | 67 | 6.244 | 22.539 | 27.815 | 1.00 | 36.76 | O |
| ATOM | 440 | N | GLU | A | 68 | 2.502 | 22.765 | 28.648 | 1.00 | 44.40 | N |
| ATOM | 441 | CA | GLU | A | 68 | 1.317 | 22.183 | 28.023 | 1.00 | 46.43 | C |
| ATOM | 442 | C | GLU | A | 68 | 1.777 | 21.448 | 26.758 | 1.00 | 46.20 | C |
| ATOM | 443 | O | GLU | A | 68 | 2.874 | 21.690 | 26.234 | 1.00 | 47.39 | O |
| ATOM | 444 | CB | GLU | A | 68 | 0.364 | 23.301 | 27.637 | 1.00 | 49.01 | C |
| ATOM | 445 | CG | GLU | A | 68 | -1.051 | 22.858 | 27.256 | 1.00 | 53.42 | C |
| ATOM | 446 | CD | GLU | A | 68 | -2.066 | 23.229 | 28.324 | 1.00 | 56.12 | C |
| ATOM | 447 | OE1 | GLU | A | 68 | -2.255 | 22.391 | 29.223 | 1.00 | 58.37 | O |
| ATOM | 448 | OE2 | GLU | A | 68 | -2.634 | 24.342 | 28.250 | 1.00 | 56.09 | O |
| ATOM | 449 | N | GLY | A | 69 | 0.957 | 20.523 | 26.262 | 1.00 | 45.44 | N |
| ATOM | 450 | CA | GLY | A | 69 | 1.228 | 19.834 | 25.021 | 1.00 | 43.62 | C |
| ATOM | 451 | C | GLY | A | 69 | 2.561 | 19.130 | 25.029 | 1.00 | 42.33 | C |
| ATOM | 452 | O | GLY | A | 69 | 2.944 | 18.429 | 25.963 | 1.00 | 43.42 | O |
| ATOM | 453 | N | LEU | A | 70 | 3.245 | 19.412 | 23.927 | 1.00 | 42.01 | N |
| ATOM | 454 | CA | LEU | A | 70 | 4.567 | 18.856 | 23.634 | 1.00 | 40.66 | C |
| ATOM | 455 | C | LEU | A | 70 | 5.570 | 19.283 | 24.688 | 1.00 | 37.48 | C |
| ATOM | 456 | O | LEU | A | 70 | 5.769 | 20.477 | 24.916 | 1.00 | 39.56 | O |
| ATOM | 457 | CB | LEU | A | 70 | 5.069 | 19.339 | 22.221 | 1.00 | 42.73 | C |
| ATOM | 458 | CG | LEU | A | 70 | 6.365 | 18.753 | 21.553 | 1.00 | 43.68 | C |
| ATOM | 459 | CD1 | LEU | A | 70 | 6.429 | 17.212 | 21.539 | 1.00 | 40.99 | C |
| ATOM | 460 | CD2 | LEU | A | 70 | 6.506 | 19.318 | 20.134 | 1.00 | 42.81 | C |
| ATOM | 461 | N | SER | A | 71 | 6.203 | 18.289 | 25.301 | 1.00 | 32.14 | N |
| ATOM | 462 | CA | SER | A | 71 | 7.187 | 18.514 | 26.330 | 1.00 | 24.30 | C |
| ATOM | 463 | C | SER | A | 71 | 8.394 | 17.653 | 26.032 | 1.00 | 20.06 | C |
| ATOM | 464 | O | SER | A | 71 | 8.282 | 16.449 | 25.900 | 1.00 | 21.51 | O |
| ATOM | 465 | CB | SER | A | 71 | 6.519 | 18.160 | 27.653 | 1.00 | 21.80 | C |
| ATOM | 466 | OG | SER | A | 71 | 7.393 | 18.171 | 28.756 | 1.00 | 17.14 | O |
| ATOM | 467 | N | ASN | A | 72 | 9.573 | 18.208 | 25.883 | 1.00 | 18.83 | N |
| ATOM | 468 | CA | ASN | A | 72 | 10.787 | 17.419 | 25.827 | 1.00 | 16.99 | C |
| ATOM | 469 | C | ASN | A | 72 | 11.079 | 16.692 | 27.083 | 1.00 | 15.54 | C |
| ATOM | 470 | O | ASN | A | 72 | 11.566 | 15.578 | 26.997 | 1.00 | 16.64 | O |
| ATOM | 471 | CB | ASN | A | 72 | 11.982 | 18.277 | 25.558 | 1.00 | 20.15 | C |
| ATOM | 472 | CG | ASN | A | 72 | 11.916 | 18.839 | 24.158 | 1.00 | 23.44 | C |
| ATOM | 473 | OD1 | ASN | A | 72 | 11.109 | 18.421 | 23.317 | 1.00 | 25.67 | O |
| ATOM | 474 | ND2 | ASN | A | 72 | 12.780 | 19.812 | 23.894 | 1.00 | 24.59 | N |
| ATOM | 475 | N | TYR | A | 73 | 10.823 | 17.309 | 28.239 | 1.00 | 15.06 | N |
| ATOM | 476 | CA | TYR | A | 73 | 10.835 | 16.579 | 29.507 | 1.00 | 15.26 | C |
| ATOM | 477 | C | TYR | A | 73 | 9.986 | 15.319 | 29.443 | 1.00 | 15.85 | C |
| ATOM | 478 | O | TYR | A | 73 | 10.538 | 14.262 | 29.740 | 1.00 | 18.32 | O |
| ATOM | 479 | CB | TYR | A | 73 | 10.315 | 17.410 | 30.733 | 1.00 | 12.75 | C |
| ATOM | 480 | CG | TYR | A | 73 | 10.760 | 16.862 | 32.082 | 1.00 | 10.27 | C |
| ATOM | 481 | CD1 | TYR | A | 73 | 11.940 | 17.306 | 32.624 | 1.00 | 11.84 | C |
| ATOM | 482 | CD2 | TYR | A | 73 | 9.993 | 15.928 | 32.769 | 1.00 | 14.03 | C |
| ATOM | 483 | CE1 | TYR | A | 73 | 12.364 | 16.827 | 33.839 | 1.00 | 12.67 | C |
| ATOM | 484 | CE2 | TYR | A | 73 | 10.412 | 15.419 | 33.979 | 1.00 | 10.24 | C |

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FIGURE 8A-19

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 485 | CZ | TYR | A | 73 | 11.592 | 15.891 | 34.491 | 1.00 | 14.02 | C |
| ATOM | 486 | OH | TYR | A | 73 | 12.042 | 15.429 | 35.703 | 1.00 | 14.54 | O |
| ATOM | 487 | N | SER | A | 74 | 8.682 | 15.323 | 29.087 | 1.00 | 18.48 | C |
| ATOM | 488 | CA | SER | A | 74 | 7.947 | 14.076 | 29.034 | 1.00 | 18.74 | N |
| ATOM | 489 | C | SER | A | 74 | 8.429 | 13.074 | 28.017 | 1.00 | 18.80 | C |
| ATOM | 490 | O | SER | A | 74 | 8.430 | 11.882 | 28.327 | 1.00 | 18.69 | O |
| ATOM | 491 | CB | SER | A | 74 | 6.434 | 14.228 | 29.002 | 1.00 | 21.96 | C |
| ATOM | 492 | OG | SER | A | 74 | 5.847 | 15.278 | 28.253 | 1.00 | 30.65 | O |
| ATOM | 493 | N | ILE | A | 75 | 8.928 | 13.522 | 26.849 | 1.00 | 18.95 | C |
| ATOM | 494 | CA | ILE | A | 75 | 9.481 | 12.602 | 25.855 | 1.00 | 17.82 | N |
| ATOM | 495 | C | ILE | A | 75 | 10.689 | 11.896 | 26.422 | 1.00 | 17.12 | C |
| ATOM | 496 | O | ILE | A | 75 | 10.679 | 10.688 | 26.557 | 1.00 | 18.03 | C |
| ATOM | 497 | CB | ILE | A | 75 | 9.750 | 13.298 | 24.460 | 1.00 | 20.42 | O |
| ATOM | 498 | CG1 | ILE | A | 75 | 8.440 | 13.885 | 23.860 | 1.00 | 19.63 | C |
| ATOM | 499 | CG2 | ILE | A | 75 | 10.327 | 12.283 | 23.471 | 1.00 | 17.30 | C |
| ATOM | 500 | CD1 | ILE | A | 75 | 8.582 | 14.604 | 22.508 | 1.00 | 23.08 | C |
| ATOM | 501 | N | ILE | A | 76 | 11.698 | 12.625 | 26.857 | 1.00 | 18.46 | C |
| ATOM | 502 | CA | ILE | A | 76 | 12.916 | 12.070 | 27.436 | 1.00 | 19.33 | N |
| ATOM | 503 | C | ILE | A | 76 | 12.622 | 11.116 | 28.592 | 1.00 | 19.01 | C |
| ATOM | 504 | O | ILE | A | 76 | 13.199 | 10.040 | 28.714 | 1.00 | 20.65 | O |
| ATOM | 505 | CB | ILE | A | 76 | 13.816 | 13.253 | 27.900 | 1.00 | 18.88 | C |
| ATOM | 506 | CG1 | ILE | A | 76 | 14.239 | 14.216 | 26.789 | 1.00 | 17.98 | C |
| ATOM | 507 | CG2 | ILE | A | 76 | 15.057 | 12.732 | 28.600 | 1.00 | 20.53 | C |
| ATOM | 508 | CD1 | ILE | A | 76 | 14.950 | 15.500 | 27.300 | 1.00 | 15.54 | C |
| ATOM | 509 | N | ASP | A | 77 | 11.643 | 11.474 | 29.412 | 1.00 | 19.90 | C |
| ATOM | 510 | CA | ASP | A | 77 | 11.226 | 10.682 | 30.562 | 1.00 | 19.93 | C |
| ATOM | 511 | C | ASP | A | 77 | 10.627 | 9.341 | 30.177 | 1.00 | 21.32 | C |
| ATOM | 512 | O | ASP | A | 77 | 10.832 | 8.318 | 30.830 | 1.00 | 21.41 | O |
| ATOM | 513 | CB | ASP | A | 77 | 10.189 | 11.524 | 31.263 | 1.00 | 21.00 | C |
| ATOM | 514 | CG | ASP | A | 77 | 9.506 | 10.808 | 32.390 | 1.00 | 23.32 | C |
| ATOM | 515 | OD1 | ASP | A | 77 | 10.211 | 10.249 | 33.204 | 1.00 | 26.02 | O |
| ATOM | 516 | OD2 | ASP | A | 77 | 8.283 | 10.750 | 32.419 | 1.00 | 24.74 | O |
| ATOM | 517 | N | LYS | A | 78 | 9.835 | 9.312 | 29.101 | 1.00 | 23.41 | N |
| ATOM | 518 | CA | LYS | A | 78 | 9.385 | 8.038 | 28.606 | 1.00 | 23.09 | C |
| ATOM | 519 | C | LYS | A | 78 | 10.529 | 7.247 | 27.975 | 1.00 | 24.61 | C |
| ATOM | 520 | O | LYS | A | 78 | 10.518 | 6.000 | 28.021 | 1.00 | 26.85 | O |
| ATOM | 521 | CB | LYS | A | 78 | 8.267 | 8.237 | 27.656 | 1.00 | 25.84 | C |
| ATOM | 522 | CG | LYS | A | 78 | 7.024 | 8.643 | 28.403 | 1.00 | 29.26 | C |
| ATOM | 523 | CD | LYS | A | 78 | 5.882 | 8.766 | 27.362 | 1.00 | 40.97 | C |
| ATOM | 524 | CE | LYS | A | 78 | 6.119 | 9.815 | 26.221 | 1.00 | 43.91 | C |
| ATOM | 525 | NZ | LYS | A | 78 | 5.056 | 9.792 | 25.229 | 1.00 | 48.24 | C |
| ATOM | 526 | N | LEU | A | 79 | 11.559 | 7.936 | 27.437 | 1.00 | 22.19 | N |
| ATOM | 527 | CA | LEU | A | 79 | 12.718 | 7.253 | 26.865 | 1.00 | 18.09 | C |
| ATOM | 528 | C | LEU | A | 79 | 13.577 | 6.757 | 27.968 | 1.00 | 16.82 | C |
| ATOM | 529 | O | LEU | A | 79 | 14.146 | 5.692 | 27.806 | 1.00 | 17.74 | O |
| ATOM | 530 | CB | LEU | A | 79 | 13.580 | 8.147 | 25.986 | 1.00 | 16.97 | C |
| ATOM | 531 | CG | LEU | A | 79 | 12.928 | 8.748 | 24.768 | 1.00 | 15.98 | C |
| ATOM | 532 | CD1 | LEU | A | 79 | 13.984 | 9.540 | 24.058 | 1.00 | 16.93 | C |
| ATOM | 533 | CD2 | LEU | A | 79 | 12.264 | 7.721 | 23.857 | 1.00 | 14.76 | C |
| ATOM | 534 | N | VAL | A | 80 | 13.609 | 7.460 | 29.101 | 1.00 | 16.48 | C |
| ATOM | 535 | CA | VAL | A | 80 | 14.352 | 6.994 | 30.249 | 1.00 | 13.79 | C |
| ATOM | 536 | C | VAL | A | 80 | 13.697 | 5.725 | 30.731 | 1.00 | 14.44 | C |
| ATOM | 537 | O | VAL | A | 80 | 14.385 | 4.763 | 31.022 | 1.00 | 14.81 | O |
| ATOM | 538 | CB | VAL | A | 80 | 14.382 | 8.054 | 31.331 | 1.00 | 17.12 | C |
| ATOM | 539 | CG1 | VAL | A | 80 | 14.937 | 7.490 | 32.631 | 1.00 | 17.65 | C |
| ATOM | 540 | CG2 | VAL | A | 80 | 15.307 | 9.189 | 30.910 | 1.00 | 13.43 | C |
| ATOM | 541 | N | ASN | A | 81 | 12.383 | 5.633 | 30.743 | 1.00 | 16.27 | C |
| ATOM | 542 | CA | ASN | A | 81 | 11.696 | 4.398 | 31.081 | 1.00 | 18.71 | C |
| ATOM | 543 | C | ASN | A | 81 | 11.852 | 3.174 | 30.176 | 1.00 | 21.49 | C |
| ATOM | 544 | O | ASN | A | 81 | 11.945 | 2.060 | 30.691 | 1.00 | 22.57 | O |

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FIGURE 8A-20

| | | | | | | | | | | | |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 545 | CB | ASN | A | 81 | 10.244 | 4.707 | 31.191 | 1.00 | 20.64 | C |
| ATOM | 546 | CG | ASN | A | 81 | 9.968 | 5.574 | 32.402 | 1.00 | 22.06 | C |
| ATOM | 547 | OD1 | ASN | A | 81 | 10.652 | 5.475 | 33.422 | 1.00 | 22.22 | N |
| ATOM | 548 | ND2 | ASN | A | 81 | 8.941 | 6.409 | 32.322 | 1.00 | 21.76 | O |
| ATOM | 549 | N | ILE | A | 82 | 11.898 | 3.339 | 28.846 | 1.00 | 21.86 | N |
| ATOM | 550 | CA | ILE | A | 82 | 12.226 | 2.270 | 27.917 | 1.00 | 23.02 | C |
| ATOM | 551 | C | ILE | A | 82 | 13.602 | 1.742 | 28.112 | 1.00 | 23.67 | C |
| ATOM | 552 | O | ILE | A | 82 | 13.728 | 0.536 | 28.067 | 1.00 | 26.85 | O |
| ATOM | 553 | CB | ILE | A | 82 | 12.089 | 2.768 | 26.497 | 1.00 | 22.79 | C |
| ATOM | 554 | CG1 | ILE | A | 82 | 10.613 | 2.757 | 26.220 | 1.00 | 23.80 | C |
| ATOM | 555 | CG2 | ILE | A | 82 | 12.854 | 1.951 | 25.474 | 1.00 | 21.98 | C |
| ATOM | 556 | CD1 | ILE | A | 82 | 10.321 | 3.659 | 25.020 | 1.00 | 27.18 | C |
| ATOM | 557 | N | VAL | A | 83 | 14.619 | 2.586 | 28.254 | 1.00 | 25.82 | N |
| ATOM | 558 | CA | VAL | A | 83 | 15.996 | 2.104 | 28.338 | 1.00 | 27.82 | C |
| ATOM | 559 | C | VAL | A | 83 | 16.212 | 1.471 | 29.706 | 1.00 | 30.01 | C |
| ATOM | 560 | O | VAL | A | 83 | 16.995 | 0.522 | 29.796 | 1.00 | 32.08 | O |
| ATOM | 561 | CB | VAL | A | 83 | 17.139 | 3.137 | 28.252 | 1.00 | 26.25 | C |
| ATOM | 562 | CG1 | VAL | A | 83 | 18.343 | 2.445 | 27.683 | 1.00 | 28.68 | C |
| ATOM | 563 | CG2 | VAL | A | 83 | 16.883 | 4.437 | 27.569 | 1.00 | 28.99 | C |
| ATOM | 564 | N | ASP | A | 84 | 15.602 | 1.983 | 30.789 | 1.00 | 30.99 | N |
| ATOM | 565 | CA | ASP | A | 84 | 15.711 | 1.384 | 32.123 | 1.00 | 34.08 | C |
| ATOM | 566 | C | ASP | A | 84 | 15.125 | -0.013 | 32.275 | 1.00 | 34.30 | C |
| ATOM | 567 | O | ASP | A | 84 | 15.666 | -0.816 | 33.035 | 1.00 | 35.01 | O |
| ATOM | 568 | CB | ASP | A | 84 | 15.148 | 2.331 | 33.189 | 1.00 | 37.32 | C |
| ATOM | 569 | CG | ASP | A | 84 | 15.909 | 3.664 | 33.316 | 1.00 | 42.03 | C |
| ATOM | 570 | OD1 | ASP | A | 84 | 16.907 | 3.865 | 32.621 | 1.00 | 43.39 | O |
| ATOM | 571 | OD2 | ASP | A | 84 | 15.496 | 4.523 | 34.107 | 1.00 | 44.86 | O |
| ATOM | 572 | N | ASP | A | 85 | 14.055 | -0.335 | 31.524 | 1.00 | 35.79 | N |
| ATOM | 573 | CA | ASP | A | 85 | 13.554 | -1.707 | 31.332 | 1.00 | 37.15 | C |
| ATOM | 574 | C | ASP | A | 85 | 14.655 | -2.665 | 30.860 | 1.00 | 34.71 | C |
| ATOM | 575 | O | ASP | A | 85 | 14.777 | -3.800 | 31.308 | 1.00 | 33.69 | O |
| ATOM | 576 | CB | ASP | A | 85 | 12.434 | -1.780 | 30.233 | 1.00 | 42.27 | C |
| ATOM | 577 | CG | ASP | A | 85 | 11.023 | -1.216 | 30.474 | 1.00 | 46.16 | C |
| ATOM | 578 | OD1 | ASP | A | 85 | 10.747 | -0.756 | 31.587 | 1.00 | 46.14 | O |
| ATOM | 579 | OD2 | ASP | A | 85 | 10.197 | -1.234 | 29.539 | 1.00 | 50.79 | O |
| ATOM | 580 | N | LEU | A | 86 | 15.437 | -2.164 | 29.904 | 1.00 | 33.83 | N |
| ATOM | 581 | CA | LEU | A | 86 | 16.527 | -2.886 | 29.288 | 1.00 | 33.71 | C |
| ATOM | 582 | C | LEU | A | 86 | 17.747 | -2.959 | 30.177 | 1.00 | 34.12 | C |
| ATOM | 583 | O | LEU | A | 86 | 18.440 | -3.965 | 30.083 | 1.00 | 34.86 | O |
| ATOM | 584 | CB | LEU | A | 86 | 16.907 | -2.260 | 27.948 | 1.00 | 31.87 | C |
| ATOM | 585 | CG | LEU | A | 86 | 15.878 | -2.198 | 26.829 | 1.00 | 30.75 | C |
| ATOM | 586 | CD1 | LEU | A | 86 | 16.383 | -1.351 | 25.699 | 1.00 | 30.54 | C |
| ATOM | 587 | CD2 | LEU | A | 86 | 15.521 | -3.581 | 26.349 | 1.00 | 29.51 | C |
| ATOM | 588 | N | VAL | A | 87 | 18.033 | -1.973 | 31.039 | 1.00 | 33.89 | N |
| ATOM | 589 | CA | VAL | A | 87 | 19.121 | -2.074 | 32.009 | 1.00 | 35.56 | C |
| ATOM | 590 | C | VAL | A | 87 | 18.933 | -3.223 | 33.039 | 1.00 | 40.73 | C |
| ATOM | 591 | O | VAL | A | 87 | 19.889 | -3.890 | 33.493 | 1.00 | 42.23 | O |
| ATOM | 592 | CB | VAL | A | 87 | 19.239 | -0.695 | 32.614 | 1.00 | 31.60 | C |
| ATOM | 593 | CG1 | VAL | A | 87 | 20.272 | -0.634 | 33.703 | 1.00 | 33.57 | C |
| ATOM | 594 | CG2 | VAL | A | 87 | 19.680 | 0.253 | 31.537 | 1.00 | 29.91 | C |
| ATOM | 595 | N | GLU | A | 88 | 17.645 | -3.484 | 33.340 | 1.00 | 44.00 | N |
| ATOM | 596 | CA | GLU | A | 88 | 17.191 | -4.563 | 34.217 | 1.00 | 47.21 | C |
| ATOM | 597 | C | GLU | A | 88 | 17.016 | -5.918 | 33.542 | 1.00 | 48.21 | C |
| ATOM | 598 | O | GLU | A | 88 | 17.359 | -6.909 | 34.169 | 1.00 | 47.84 | O |
| ATOM | 599 | CB | GLU | A | 88 | 15.868 | -4.200 | 34.886 | 1.00 | 49.05 | C |
| ATOM | 600 | CG | GLU | A | 88 | 15.877 | -2.952 | 35.772 | 1.00 | 52.09 | C |
| ATOM | 601 | CD | GLU | A | 88 | 16.809 | -3.020 | 36.976 | 1.00 | 53.70 | C |
| ATOM | 602 | OE1 | GLU | A | 88 | 16.608 | -3.858 | 37.861 | 1.00 | 55.01 | O |
| ATOM | 603 | OE2 | GLU | A | 88 | 17.744 | -2.221 | 37.020 | 1.00 | 54.23 | O |
| ATOM | 604 | N | CYS | A | 89 | 16.475 | -6.018 | 32.311 | 1.00 | 50.79 | N |

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FIGURE 8A-21

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 605 | CA | CYS | A | 89 | 16.489 | -7.244 | 31.503 | 1.00 | 54.51 | C |
| ATOM | 606 | C | CYS | A | 89 | 17.952 | -7.703 | 31.459 | 1.00 | 55.09 | O |
| ATOM | 607 | O | CYS | A | 89 | 18.231 | -8.791 | 31.961 | 1.00 | 57.42 | S |
| ATOM | 608 | CB | CYS | A | 89 | 15.903 | -6.972 | 30.078 | 1.00 | 57.17 | N |
| ATOM | 609 | SG | CYS | A | 89 | 15.060 | -8.280 | 29.096 | 1.00 | 64.80 | C |
| ATOM | 610 | N | VAL | A | 90 | 18.890 | -6.838 | 31.002 | 1.00 | 55.69 | O |
| ATOM | 611 | CA | VAL | A | 90 | 20.357 | -7.027 | 31.060 | 1.00 | 55.91 | C |
| ATOM | 612 | C | VAL | A | 90 | 20.906 | -7.397 | 32.450 | 1.00 | 57.84 | O |
| ATOM | 613 | O | VAL | A | 90 | 22.014 | -7.924 | 32.546 | 1.00 | 58.27 | C |
| ATOM | 614 | CB | VAL | A | 90 | 21.074 | -5.738 | 30.480 | 1.00 | 53.45 | O |
| ATOM | 615 | CG1 | VAL | A | 90 | 22.542 | -5.564 | 30.824 | 1.00 | 52.76 | C |
| ATOM | 616 | CG2 | VAL | A | 90 | 20.965 | -5.689 | 28.978 | 1.00 | 50.05 | O |
| ATOM | 617 | N | LYS | A | 91 | 20.212 | -7.128 | 33.558 | 1.00 | 59.29 | C |
| ATOM | 618 | CA | LYS | A | 91 | 20.556 | -7.785 | 34.810 | 1.00 | 62.11 | O |
| ATOM | 619 | C | LYS | A | 91 | 19.865 | -9.163 | 34.996 | 1.00 | 63.85 | C |
| ATOM | 620 | O | LYS | A | 91 | 20.517 | -10.061 | 35.533 | 1.00 | 66.48 | O |
| ATOM | 621 | CB | LYS | A | 91 | 20.305 | -6.837 | 35.993 | 1.00 | 61.39 | C |
| ATOM | 622 | N | SER | A | 104 | 36.757 | 4.074 | 31.300 | 1.00 | 64.71 | N |
| ATOM | 623 | CA | SER | A | 104 | 36.147 | 4.043 | 29.974 | 1.00 | 64.00 | C |
| ATOM | 624 | C | SER | A | 104 | 34.723 | 3.416 | 29.904 | 1.00 | 61.57 | O |
| ATOM | 625 | O | SER | A | 104 | 34.321 | 2.749 | 30.871 | 1.00 | 62.78 | C |
| ATOM | 626 | CB | SER | A | 104 | 37.147 | 3.441 | 28.919 | 1.00 | 65.90 | O |
| ATOM | 627 | OG | SER | A | 104 | 38.150 | 4.399 | 28.533 | 1.00 | 67.30 | C |
| ATOM | 628 | N | PRO | A | 105 | 33.891 | 3.576 | 28.842 | 1.00 | 57.26 | O |
| ATOM | 629 | CA | PRO | A | 105 | 34.173 | 4.332 | 27.635 | 1.00 | 53.19 | C |
| ATOM | 630 | C | PRO | A | 105 | 34.452 | 5.801 | 27.827 | 1.00 | 51.76 | O |
| ATOM | 631 | O | PRO | A | 105 | 34.107 | 6.397 | 28.848 | 1.00 | 53.30 | C |
| ATOM | 632 | CB | PRO | A | 105 | 32.968 | 4.091 | 26.813 | 1.00 | 51.85 | O |
| ATOM | 633 | CG | PRO | A | 105 | 31.869 | 3.765 | 27.755 | 1.00 | 53.45 | C |
| ATOM | 634 | CD | PRO | A | 105 | 32.618 | 2.880 | 28.698 | 1.00 | 55.74 | O |
| ATOM | 635 | N | GLU | A | 106 | 35.242 | 6.296 | 26.875 | 1.00 | 50.80 | C |
| ATOM | 636 | CA | GLU | A | 106 | 35.584 | 7.700 | 26.790 | 1.00 | 47.97 | N |
| ATOM | 637 | C | GLU | A | 106 | 34.332 | 8.435 | 26.350 | 1.00 | 44.14 | C |
| ATOM | 638 | O | GLU | A | 106 | 33.684 | 8.006 | 25.400 | 1.00 | 42.91 | O |
| ATOM | 639 | CB | GLU | A | 106 | 36.796 | 7.970 | 25.858 | 1.00 | 51.71 | C |
| ATOM | 640 | CG | GLU | A | 106 | 36.873 | 7.196 | 24.509 | 1.00 | 57.13 | O |
| ATOM | 641 | CD | GLU | A | 106 | 38.045 | 6.192 | 24.389 | 1.00 | 60.78 | C |
| ATOM | 642 | OE1 | GLU | A | 106 | 38.141 | 5.251 | 25.189 | 1.00 | 61.59 | O |
| ATOM | 643 | OE2 | GLU | A | 106 | 38.874 | 6.338 | 23.482 | 1.00 | 63.52 | O |
| ATOM | 644 | N | PRO | A | 107 | 33.936 | 9.481 | 27.092 | 1.00 | 41.02 | N |
| ATOM | 645 | CA | PRO | A | 107 | 32.846 | 10.386 | 26.770 | 1.00 | 38.74 | C |
| ATOM | 646 | C | PRO | A | 107 | 33.069 | 11.190 | 25.517 | 1.00 | 37.93 | O |
| ATOM | 647 | O | PRO | A | 107 | 34.148 | 11.749 | 25.271 | 1.00 | 40.00 | C |
| ATOM | 648 | CB | PRO | A | 107 | 32.764 | 11.292 | 27.970 | 1.00 | 39.85 | O |
| ATOM | 649 | CG | PRO | A | 107 | 34.162 | 11.290 | 28.542 | 1.00 | 40.91 | C |
| ATOM | 650 | CD | PRO | A | 107 | 34.522 | 9.832 | 28.384 | 1.00 | 41.30 | O |
| ATOM | 651 | N | ARG | A | 108 | 32.000 | 11.208 | 24.724 | 1.00 | 35.40 | N |
| ATOM | 652 | CA | ARG | A | 108 | 32.006 | 11.864 | 23.436 | 1.00 | 33.34 | C |
| ATOM | 653 | C | ARG | A | 108 | 30.766 | 12.722 | 23.318 | 1.00 | 29.75 | O |
| ATOM | 654 | O | ARG | A | 108 | 29.727 | 12.347 | 23.867 | 1.00 | 29.55 | C |
| ATOM | 655 | CB | ARG | A | 108 | 32.102 | 10.859 | 22.297 | 1.00 | 35.14 | O |
| ATOM | 656 | CG | ARG | A | 108 | 33.480 | 10.219 | 22.313 | 1.00 | 39.55 | C |
| ATOM | 657 | CD | ARG | A | 108 | 33.734 | 9.386 | 21.057 | 1.00 | 44.05 | O |
| ATOM | 658 | NE | ARG | A | 108 | 34.715 | 8.324 | 21.284 | 1.00 | 45.36 | C |
| ATOM | 659 | CZ | ARG | A | 108 | 34.965 | 7.376 | 20.373 | 1.00 | 45.18 | N |
| ATOM | 660 | NH1 | ARG | A | 108 | 34.481 | 7.446 | 19.142 | 1.00 | 46.89 | C |
| ATOM | 661 | NH2 | ARG | A | 108 | 35.679 | 6.306 | 20.712 | 1.00 | 46.89 | N |
| ATOM | 662 | N | LEU | A | 109 | 30.932 | 13.877 | 22.650 | 1.00 | 26.42 | N |
| ATOM | 663 | CA | LEU | A | 109 | 29.833 | 14.770 | 22.334 | 1.00 | 25.17 | C |
| ATOM | 664 | C | LEU | A | 109 | 29.126 | 14.453 | 21.020 | 1.00 | 25.96 | C |

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FIGURE 8A-22

| | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 665 | O | LEU | A | 109 | 29.774 | 14.229 | 20.002 | 1.00 | 26.43 |
| ATOM | 666 | CB | LEU | A | 109 | 30.316 | 16.182 | 22.280 | 1.00 | 24.30 |
| ATOM | 667 | CG | LEU | A | 109 | 31.003 | 16.770 | 23.483 | 1.00 | 25.72 |
| ATOM | 668 | CD1 | LEU | A | 109 | 31.426 | 18.185 | 23.137 | 1.00 | 25.28 |
| ATOM | 669 | CD2 | LEU | A | 109 | 30.097 | 16.820 | 24.677 | 1.00 | 25.67 |
| ATOM | 670 | N | PHE | A | 110 | 27.794 | 14.427 | 20.988 | 1.00 | 24.52 |
| ATOM | 671 | CA | PHE | A | 110 | 27.019 | 14.004 | 19.822 | 1.00 | 22.36 |
| ATOM | 672 | C | PHE | A | 110 | 25.996 | 15.079 | 19.586 | 1.00 | 21.47 |
| ATOM | 673 | O | PHE | A | 110 | 25.618 | 15.777 | 20.525 | 1.00 | 21.05 |
| ATOM | 674 | CB | PHE | A | 110 | 26.227 | 12.725 | 20.075 | 1.00 | 21.69 |
| ATOM | 675 | CG | PHE | A | 110 | 27.133 | 11.561 | 20.318 | 1.00 | 23.01 |
| ATOM | 676 | CD1 | PHE | A | 110 | 27.676 | 10.892 | 19.238 | 1.00 | 24.43 |
| ATOM | 677 | CD2 | PHE | A | 110 | 27.506 | 11.243 | 21.597 | 1.00 | 21.68 |
| ATOM | 678 | CE1 | PHE | A | 110 | 28.614 | 9.897 | 19.463 | 1.00 | 24.92 |
| ATOM | 679 | CE2 | PHE | A | 110 | 28.460 | 10.282 | 21.798 | 1.00 | 22.08 |
| ATOM | 680 | CZ | PHE | A | 110 | 29.017 | 9.597 | 20.746 | 1.00 | 23.51 |
| ATOM | 681 | N | THR | A | 111 | 25.557 | 15.239 | 18.339 | 1.00 | 20.40 |
| ATOM | 682 | CA | THR | A | 111 | 24.422 | 16.102 | 18.047 | 1.00 | 19.58 |
| ATOM | 683 | C | THR | A | 111 | 23.175 | 15.367 | 18.473 | 1.00 | 15.81 |
| ATOM | 684 | O | THR | A | 111 | 23.239 | 14.150 | 18.603 | 1.00 | 18.63 |
| ATOM | 685 | CB | THR | A | 111 | 24.305 | 16.421 | 16.578 | 1.00 | 19.96 |
| ATOM | 686 | OG1 | THR | A | 111 | 24.145 | 15.178 | 15.907 | 1.00 | 21.91 |
| ATOM | 687 | CG2 | THR | A | 111 | 25.487 | 17.252 | 16.118 | 1.00 | 23.08 |
| ATOM | 688 | N | PRO | A | 112 | 22.030 | 15.982 | 18.688 | 1.00 | 15.89 |
| ATOM | 689 | CA | PRO | A | 112 | 20.783 | 15.254 | 18.984 | 1.00 | 16.41 |
| ATOM | 690 | C | PRO | A | 112 | 20.500 | 14.089 | 18.025 | 1.00 | 17.10 |
| ATOM | 691 | O | PRO | A | 112 | 20.329 | 12.954 | 18.431 | 1.00 | 18.32 |
| ATOM | 692 | CB | PRO | A | 112 | 19.794 | 16.375 | 18.870 | 1.00 | 13.89 |
| ATOM | 693 | CG | PRO | A | 112 | 20.581 | 17.559 | 19.386 | 1.00 | 14.36 |
| ATOM | 694 | CD | PRO | A | 112 | 21.876 | 17.424 | 18.685 | 1.00 | 12.46 |
| ATOM | 695 | N | GLU | A | 113 | 20.564 | 14.321 | 16.728 | 1.00 | 20.22 |
| ATOM | 696 | CA | GLU | A | 113 | 20.393 | 13.303 | 15.737 | 1.00 | 24.11 |
| ATOM | 697 | C | GLU | A | 113 | 21.371 | 12.143 | 15.864 | 1.00 | 24.55 |
| ATOM | 698 | O | GLU | A | 113 | 20.963 | 10.982 | 15.866 | 1.00 | 25.38 |
| ATOM | 699 | CB | GLU | A | 113 | 20.539 | 13.991 | 14.420 | 1.00 | 29.66 |
| ATOM | 700 | CG | GLU | A | 113 | 20.432 | 13.029 | 13.250 | 1.00 | 41.26 |
| ATOM | 701 | CD | GLU | A | 113 | 21.253 | 13.476 | 12.042 | 1.00 | 49.84 |
| ATOM | 702 | OE1 | GLU | A | 113 | 22.475 | 13.694 | 12.197 | 1.00 | 52.84 |
| ATOM | 703 | OE2 | GLU | A | 113 | 20.662 | 13.586 | 10.949 | 1.00 | 55.78 |
| ATOM | 704 | N | GLU | A | 114 | 22.663 | 12.384 | 16.033 | 1.00 | 24.48 |
| ATOM | 705 | CA | GLU | A | 114 | 23.594 | 11.291 | 16.198 | 1.00 | 22.26 |
| ATOM | 706 | C | GLU | A | 114 | 23.398 | 10.486 | 17.471 | 1.00 | 22.80 |
| ATOM | 707 | O | GLU | A | 114 | 23.564 | 9.256 | 17.494 | 1.00 | 23.87 |
| ATOM | 708 | CB | GLU | A | 114 | 24.979 | 11.857 | 16.198 | 1.00 | 26.15 |
| ATOM | 709 | CG | GLU | A | 114 | 25.362 | 12.534 | 14.897 | 1.00 | 32.62 |
| ATOM | 710 | CD | GLU | A | 114 | 26.719 | 13.225 | 15.002 | 1.00 | 38.61 |
| ATOM | 711 | OE1 | GLU | A | 114 | 26.860 | 14.093 | 15.867 | 1.00 | 41.67 |
| ATOM | 712 | OE2 | GLU | A | 114 | 27.646 | 12.893 | 14.242 | 1.00 | 42.28 |
| ATOM | 713 | N | PHE | A | 115 | 23.035 | 11.181 | 18.558 | 1.00 | 21.59 |
| ATOM | 714 | CA | PHE | A | 115 | 22.812 | 10.544 | 19.850 | 1.00 | 19.30 |
| ATOM | 715 | C | PHE | A | 115 | 21.601 | 9.645 | 19.667 | 1.00 | 17.06 |
| ATOM | 716 | O | PHE | A | 115 | 21.555 | 8.527 | 20.165 | 1.00 | 17.46 |
| ATOM | 717 | CB | PHE | A | 115 | 22.586 | 11.623 | 20.972 | 1.00 | 16.68 |
| ATOM | 718 | CG | PHE | A | 115 | 22.148 | 11.018 | 22.298 | 1.00 | 13.67 |
| ATOM | 719 | CD1 | PHE | A | 115 | 20.820 | 10.679 | 22.520 | 1.00 | 15.42 |
| ATOM | 720 | CD2 | PHE | A | 115 | 23.081 | 10.752 | 23.261 | 1.00 | 15.56 |
| ATOM | 721 | CE1 | PHE | A | 115 | 20.412 | 10.003 | 23.650 | 1.00 | 16.48 |
| ATOM | 722 | CE2 | PHE | A | 115 | 22.674 | 10.136 | 24.429 | 1.00 | 17.36 |
| ATOM | 723 | CZ | PHE | A | 115 | 21.351 | 9.750 | 24.617 | 1.00 | 18.29 |
| ATOM | 724 | N | PHE | A | 116 | 20.581 | 10.135 | 18.981 | 1.00 | 18.67 |

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FIGURE 8A-23

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 725 | CA | PHE | A | 116 | 19.401 | 9.327 | 18.860 | 1.00 | 18.51 | C |
| ATOM | 726 | C | PHE | A | 116 | 19.510 | 8.196 | 17.854 | 1.00 | 22.03 | C |
| ATOM | 727 | O | PHE | A | 116 | 18.768 | 7.213 | 17.892 | 1.00 | 22.83 | O |
| ATOM | 728 | CB | PHE | A | 116 | 18.204 | 10.195 | 18.687 | 1.00 | 19.13 | C |
| ATOM | 729 | CG | PHE | A | 116 | 17.735 | 10.764 | 20.021 | 1.00 | 19.41 | C |
| ATOM | 730 | CD1 | PHE | A | 116 | 17.159 | 9.924 | 20.952 | 1.00 | 19.08 | C |
| ATOM | 731 | CD2 | PHE | A | 116 | 17.991 | 12.079 | 20.343 | 1.00 | 19.60 | C |
| ATOM | 732 | CE1 | PHE | A | 116 | 16.911 | 10.381 | 22.214 | 1.00 | 18.67 | C |
| ATOM | 733 | CE2 | PHE | A | 116 | 17.747 | 12.528 | 21.619 | 1.00 | 21.95 | C |
| ATOM | 734 | CZ | PHE | A | 116 | 17.218 | 11.674 | 22.550 | 1.00 | 19.99 | C |
| ATOM | 735 | N | ARG | A | 117 | 20.510 | 8.249 | 16.986 | 1.00 | 22.43 | N |
| ATOM | 736 | CA | ARG | A | 117 | 20.822 | 7.134 | 16.123 | 1.00 | 21.98 | C |
| ATOM | 737 | C | ARG | A | 117 | 21.453 | 6.076 | 16.971 | 1.00 | 19.70 | C |
| ATOM | 738 | O | ARG | A | 117 | 21.039 | 4.946 | 16.841 | 1.00 | 22.56 | O |
| ATOM | 739 | CB | ARG | A | 117 | 21.769 | 7.623 | 15.052 | 1.00 | 27.63 | C |
| ATOM | 740 | CG | ARG | A | 117 | 22.329 | 6.596 | 14.082 | 1.00 | 36.33 | C |
| ATOM | 741 | CD | ARG | A | 117 | 23.135 | 7.255 | 12.971 | 1.00 | 43.02 | C |
| ATOM | 742 | NE | ARG | A | 117 | 22.296 | 8.207 | 12.239 | 1.00 | 49.61 | N |
| ATOM | 743 | CZ | ARG | A | 117 | 22.704 | 9.468 | 12.008 | 1.00 | 54.02 | C |
| ATOM | 744 | NH1 | ARG | A | 117 | 23.915 | 9.867 | 12.474 | 1.00 | 53.58 | N |
| ATOM | 745 | NH2 | ARG | A | 117 | 21.899 | 10.314 | 11.313 | 1.00 | 53.56 | N |
| ATOM | 746 | N | ILE | A | 118 | 22.394 | 6.348 | 17.874 | 1.00 | 19.56 | N |
| ATOM | 747 | CA | ILE | A | 118 | 22.944 | 5.328 | 18.746 | 1.00 | 18.66 | C |
| ATOM | 748 | C | ILE | A | 118 | 21.888 | 4.776 | 19.673 | 1.00 | 19.62 | C |
| ATOM | 749 | O | ILE | A | 118 | 21.887 | 3.579 | 19.933 | 1.00 | 21.23 | O |
| ATOM | 750 | CB | ILE | A | 118 | 24.054 | 5.970 | 19.533 | 1.00 | 21.60 | C |
| ATOM | 751 | CG1 | ILE | A | 118 | 25.121 | 6.479 | 18.593 | 1.00 | 22.63 | C |
| ATOM | 752 | CG2 | ILE | A | 118 | 24.665 | 5.002 | 20.534 | 1.00 | 22.20 | C |
| ATOM | 753 | CD1 | ILE | A | 118 | 26.178 | 7.330 | 19.285 | 1.00 | 23.90 | C |
| ATOM | 754 | N | PHE | A | 119 | 20.971 | 5.619 | 20.180 | 1.00 | 20.06 | N |
| ATOM | 755 | CA | PHE | A | 119 | 19.827 | 5.124 | 20.943 | 1.00 | 21.07 | C |
| ATOM | 756 | C | PHE | A | 119 | 18.940 | 4.182 | 20.141 | 1.00 | 21.06 | C |
| ATOM | 757 | O | PHE | A | 119 | 18.720 | 3.075 | 20.600 | 1.00 | 22.31 | O |
| ATOM | 758 | CB | PHE | A | 119 | 19.001 | 6.253 | 21.590 | 1.00 | 18.55 | C |
| ATOM | 759 | CG | PHE | A | 119 | 17.726 | 5.856 | 22.342 | 1.00 | 18.55 | C |
| ATOM | 760 | CD1 | PHE | A | 119 | 16.517 | 5.708 | 21.673 | 1.00 | 17.37 | C |
| ATOM | 761 | CD2 | PHE | A | 119 | 17.736 | 5.715 | 23.718 | 1.00 | 21.09 | C |
| ATOM | 762 | CE1 | PHE | A | 119 | 15.348 | 5.439 | 22.351 | 1.00 | 16.37 | C |
| ATOM | 763 | CE2 | PHE | A | 119 | 16.555 | 5.448 | 24.404 | 1.00 | 19.97 | C |
| ATOM | 764 | CZ | PHE | A | 119 | 15.369 | 5.311 | 23.721 | 1.00 | 19.81 | C |
| ATOM | 765 | N | ASN | A | 120 | 18.426 | 4.507 | 18.957 | 1.00 | 22.51 | N |
| ATOM | 766 | CA | ASN | A | 120 | 17.567 | 3.577 | 18.222 | 1.00 | 23.92 | C |
| ATOM | 767 | C | ASN | A | 120 | 18.284 | 2.316 | 17.841 | 1.00 | 25.82 | C |
| ATOM | 768 | O | ASN | A | 120 | 17.653 | 1.274 | 17.841 | 1.00 | 26.73 | O |
| ATOM | 769 | CB | ASN | A | 120 | 16.912 | 4.179 | 16.996 | 1.00 | 20.96 | C |
| ATOM | 770 | CG | ASN | A | 120 | 15.857 | 5.195 | 17.377 | 1.00 | 24.90 | C |
| ATOM | 771 | OD1 | ASN | A | 120 | 14.852 | 4.877 | 18.020 | 1.00 | 30.44 | O |
| ATOM | 772 | ND2 | ASN | A | 120 | 16.044 | 6.458 | 17.023 | 1.00 | 26.09 | N |
| ATOM | 773 | N | ARG | A | 121 | 19.605 | 2.390 | 17.632 | 1.00 | 29.29 | N |
| ATOM | 774 | CA | ARG | A | 121 | 20.447 | 1.234 | 17.314 | 1.00 | 32.15 | C |
| ATOM | 775 | C | ARG | A | 121 | 20.686 | 0.283 | 18.503 | 1.00 | 32.13 | C |
| ATOM | 776 | O | ARG | A | 121 | 20.652 | -0.949 | 18.369 | 1.00 | 32.27 | O |
| ATOM | 777 | CB | ARG | A | 121 | 21.752 | 1.846 | 16.891 | 1.00 | 36.26 | C |
| ATOM | 778 | CG | ARG | A | 121 | 22.606 | 0.988 | 16.001 | 1.00 | 42.80 | C |
| ATOM | 779 | CD | ARG | A | 121 | 24.066 | 1.304 | 16.288 | 1.00 | 45.46 | C |
| ATOM | 780 | NE | ARG | A | 121 | 24.730 | 0.026 | 16.469 | 1.00 | 49.59 | N |
| ATOM | 781 | CZ | ARG | A | 121 | 25.603 | -0.473 | 15.599 | 1.00 | 47.62 | C |
| ATOM | 782 | NH1 | ARG | A | 121 | 26.106 | 0.291 | 14.622 | 1.00 | 50.56 | N |
| ATOM | 783 | NH2 | ARG | A | 121 | 25.907 | -1.764 | 15.692 | 1.00 | 41.39 | N |
| ATOM | 784 | N | SER | A | 122 | 20.925 | 0.856 | 19.695 | 1.00 | 29.65 | N |

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FIGURE 8A-24

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 785 | CA | SER | A | 122 | 20.981 | 0.077 | 20.908 | 1.00 | 27.73 | C |
| ATOM | 786 | C | SER | A | 122 | 19.643 | -0.555 | 21.201 | 1.00 | 27.23 | C |
| ATOM | 787 | O | SER | A | 122 | 19.603 | -1.652 | 21.716 | 1.00 | 28.27 | C |
| ATOM | 788 | CB | SER | A | 122 | 21.388 | 0.942 | 22.071 | 1.00 | 25.31 | C |
| ATOM | 789 | OG | SER | A | 122 | 22.619 | 1.543 | 21.726 | 1.00 | 25.19 | C |
| ATOM | 790 | N | ILE | A | 123 | 18.530 | 0.087 | 20.884 | 1.00 | 29.27 | C |
| ATOM | 791 | CA | ILE | A | 123 | 17.210 | -0.453 | 21.140 | 1.00 | 31.25 | C |
| ATOM | 792 | C | ILE | A | 123 | 16.972 | -1.618 | 20.207 | 1.00 | 32.43 | C |
| ATOM | 793 | O | ILE | A | 123 | 16.522 | -2.672 | 20.637 | 1.00 | 32.75 | C |
| ATOM | 794 | CB | ILE | A | 123 | 16.129 | 0.661 | 20.973 | 1.00 | 33.20 | C |
| ATOM | 795 | CG1 | ILE | A | 123 | 16.103 | 1.685 | 22.130 | 1.00 | 35.29 | C |
| ATOM | 796 | CG2 | ILE | A | 123 | 14.739 | 0.181 | 20.629 | 1.00 | 33.87 | C |
| ATOM | 797 | CD1 | ILE | A | 123 | 16.243 | 1.313 | 23.627 | 1.00 | 32.91 | C |
| ATOM | 798 | N | ASP | A | 124 | 17.325 | -1.466 | 18.937 | 1.00 | 35.41 | C |
| ATOM | 799 | CA | ASP | A | 124 | 17.064 | -2.502 | 17.973 | 1.00 | 38.41 | N |
| ATOM | 800 | C | ASP | A | 124 | 17.902 | -3.728 | 18.170 | 1.00 | 38.55 | C |
| ATOM | 801 | O | ASP | A | 124 | 17.386 | -4.820 | 17.960 | 1.00 | 39.71 | C |
| ATOM | 802 | CB | ASP | A | 124 | 17.074 | -1.951 | 16.562 | 1.00 | 43.19 | C |
| ATOM | 803 | CG | ASP | A | 124 | 15.763 | -1.179 | 16.387 | 1.00 | 51.27 | C |
| ATOM | 804 | OD1 | ASP | A | 124 | 14.700 | -1.790 | 16.620 | 1.00 | 56.07 | C |
| ATOM | 805 | OD2 | ASP | A | 124 | 15.784 | 0.020 | 16.039 | 1.00 | 54.65 | O |
| ATOM | 806 | N | ALA | A | 125 | 19.102 | -3.546 | 18.739 | 1.00 | 37.63 | O |
| ATOM | 807 | CA | ALA | A | 125 | 20.039 | -4.621 | 18.983 | 1.00 | 37.10 | N |
| ATOM | 808 | C | ALA | A | 125 | 19.555 | -5.682 | 19.944 | 1.00 | 39.02 | C |
| ATOM | 809 | O | ALA | A | 125 | 20.250 | -6.667 | 20.151 | 1.00 | 40.94 | O |
| ATOM | 810 | CB | ALA | A | 125 | 21.321 | -4.035 | 19.500 | 1.00 | 35.16 | C |
| ATOM | 811 | N | PHE | A | 126 | 18.374 | -5.538 | 20.549 | 1.00 | 41.54 | C |
| ATOM | 812 | CA | PHE | A | 126 | 17.774 | -6.599 | 21.363 | 1.00 | 45.13 | N |
| ATOM | 813 | C | PHE | A | 126 | 16.837 | -7.482 | 20.578 | 1.00 | 47.39 | C |
| ATOM | 814 | O | PHE | A | 126 | 16.711 | -8.660 | 20.900 | 1.00 | 48.19 | O |
| ATOM | 815 | CB | PHE | A | 126 | 16.971 | -6.099 | 22.571 | 1.00 | 45.19 | C |
| ATOM | 816 | CG | PHE | A | 126 | 17.791 | -5.456 | 23.683 | 1.00 | 44.53 | C |
| ATOM | 817 | CD1 | PHE | A | 126 | 18.239 | -4.150 | 23.568 | 1.00 | 43.63 | C |
| ATOM | 818 | CD2 | PHE | A | 126 | 18.073 | -6.184 | 24.815 | 1.00 | 44.69 | C |
| ATOM | 819 | CE1 | PHE | A | 126 | 18.960 | -3.565 | 24.576 | 1.00 | 41.80 | C |
| ATOM | 820 | CE2 | PHE | A | 126 | 18.800 | -5.597 | 25.822 | 1.00 | 43.70 | C |
| ATOM | 821 | CZ | PHE | A | 126 | 19.238 | -4.295 | 25.700 | 1.00 | 43.96 | C |
| ATOM | 822 | N | LYS | A | 127 | 16.128 | -6.898 | 19.600 | 1.00 | 50.61 | N |
| ATOM | 823 | CA | LYS | A | 127 | 15.283 | -7.656 | 18.679 | 1.00 | 53.56 | C |
| ATOM | 824 | C | LYS | A | 127 | 16.149 | -8.640 | 17.856 | 1.00 | 55.43 | C |
| ATOM | 825 | O | LYS | A | 127 | 16.038 | -9.876 | 17.922 | 1.00 | 57.14 | O |
| ATOM | 826 | CB | LYS | A | 127 | 14.546 | -6.638 | 17.764 | 1.00 | 51.56 | C |
| ATOM | 827 | N | ASP | A | 128 | 17.077 | -8.036 | 17.105 | 1.00 | 57.96 | N |
| ATOM | 828 | CA | ASP | A | 128 | 18.105 | -8.734 | 16.356 | 1.00 | 59.25 | C |
| ATOM | 829 | C | ASP | A | 128 | 19.292 | -9.249 | 17.190 | 1.00 | 59.16 | C |
| ATOM | 830 | O | ASP | A | 128 | 20.461 | -8.894 | 17.008 | 1.00 | 58.89 | C |
| ATOM | 831 | CB | ASP | A | 128 | 18.492 | -7.915 | 15.062 | 1.00 | 61.00 | C |
| ATOM | 832 | CG | ASP | A | 128 | 18.868 | -6.421 | 15.036 | 1.00 | 61.70 | C |
| ATOM | 833 | OD1 | ASP | A | 128 | 20.024 | -6.078 | 15.330 | 1.00 | 63.63 | C |
| ATOM | 834 | OD2 | ASP | A | 128 | 18.015 | -5.603 | 14.667 | 1.00 | 61.66 | O |
| ATOM | 835 | N | PHE | A | 129 | 18.967 | -10.151 | 18.118 | 1.00 | 59.49 | O |
| ATOM | 836 | CA | PHE | A | 129 | 19.969 | -10.719 | 19.002 | 1.00 | 61.20 | N |
| ATOM | 837 | C | PHE | A | 129 | 20.411 | -12.103 | 18.503 | 1.00 | 61.55 | C |
| ATOM | 838 | O | PHE | A | 129 | 19.596 | -12.979 | 18.179 | 1.00 | 61.67 | C |
| ATOM | 839 | CB | PHE | A | 129 | 19.410 | -10.801 | 20.440 | 1.00 | 64.40 | C |
| ATOM | 840 | CG | PHE | A | 129 | 20.326 | -10.282 | 21.561 | 1.00 | 67.62 | C |
| ATOM | 841 | CD1 | PHE | A | 129 | 21.642 | -10.721 | 21.686 | 1.00 | 68.55 | C |
| ATOM | 842 | CD2 | PHE | A | 129 | 19.847 | -9.338 | 22.473 | 1.00 | 69.51 | C |
| ATOM | 843 | CE1 | PHE | A | 129 | 22.464 | -10.192 | 22.672 | 1.00 | 68.84 | C |
| ATOM | 844 | CE2 | PHE | A | 129 | 20.665 | -8.823 | 23.472 | 1.00 | 68.79 | C |

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FIGURE 8A-25

| | | | | | | | | | | | |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|---|
| ATOM | 845 | CZ | PHE | A | 129 | 21.976 | -9.245 | 23.561 | 1.00 | 69.80 | C |
| ATOM | 846 | N | VAL | A | 130 | 21.737 | -12.294 | 18.417 | 1.00 | 60.68 | N |
| ATOM | 847 | CA | VAL | A | 130 | 22.337 | -13.577 | 18.041 | 1.00 | 60.72 | C |
| ATOM | 848 | C | VAL | A | 130 | 23.459 | -13.949 | 19.040 | 1.00 | 59.57 | C |
| ATOM | 849 | O | VAL | A | 130 | 24.157 | -13.076 | 19.597 | 1.00 | 58.08 | O |
| ATOM | 850 | CB | VAL | A | 130 | 22.937 | -13.560 | 16.582 | 1.00 | 60.98 | C |
| ATOM | 851 | CG1 | VAL | A | 130 | 23.051 | -15.001 | 16.068 | 1.00 | 60.93 | C |
| ATOM | 852 | CG2 | VAL | A | 130 | 22.229 | -12.635 | 15.579 | 1.00 | 58.32 | C |
| ATOM | 853 | N | VAL | A | 131 | 23.635 | -15.277 | 19.213 | 1.00 | 57.03 | N |
| ATOM | 854 | CA | VAL | A | 131 | 24.634 | -15.872 | 20.101 | 1.00 | 54.98 | C |
| ATOM | 855 | C | VAL | A | 131 | 26.059 | -15.336 | 19.950 | 1.00 | 53.17 | C |
| ATOM | 856 | O | VAL | A | 131 | 26.547 | -15.173 | 18.839 | 1.00 | 51.72 | O |
| ATOM | 857 | CB | VAL | A | 131 | 24.563 | -17.411 | 19.950 | 1.00 | 55.34 | C |
| ATOM | 858 | CG1 | VAL | A | 131 | 25.611 | -18.162 | 20.780 | 1.00 | 55.30 | C |
| ATOM | 859 | CG2 | VAL | A | 131 | 23.145 | -17.893 | 20.297 | 1.00 | 54.41 | C |
| ATOM | 860 | N | ALA | A | 132 | 26.660 | -15.027 | 21.117 | 1.00 | 52.91 | N |
| ATOM | 861 | CA | ALA | A | 132 | 28.022 | -14.512 | 21.293 | 1.00 | 52.69 | C |
| ATOM | 862 | C | ALA | A | 132 | 29.161 | -15.433 | 20.860 | 1.00 | 53.47 | C |
| ATOM | 863 | O | ALA | A | 132 | 30.250 | -15.019 | 20.445 | 1.00 | 52.96 | O |
| ATOM | 864 | CB | ALA | A | 132 | 28.268 | -14.176 | 22.771 | 1.00 | 48.84 | C |
| ATOM | 865 | N | SER | A | 133 | 28.899 | -16.725 | 21.000 | 1.00 | 55.81 | N |
| ATOM | 866 | CA | SER | A | 133 | 29.812 | -17.748 | 20.533 | 1.00 | 58.09 | C |
| ATOM | 867 | C | SER | A | 133 | 29.744 | -17.881 | 19.005 | 1.00 | 59.46 | C |
| ATOM | 868 | O | SER | A | 133 | 30.726 | -18.259 | 18.343 | 1.00 | 61.98 | O |
| ATOM | 869 | CB | SER | A | 133 | 29.348 | -19.047 | 21.161 | 1.00 | 59.31 | C |
| ATOM | 870 | N | GLU | A | 134 | 28.556 | -17.536 | 18.469 | 1.00 | 58.84 | N |
| ATOM | 871 | CA | GLU | A | 134 | 28.251 | -17.530 | 17.031 | 1.00 | 57.10 | C |
| ATOM | 872 | C | GLU | A | 134 | 28.550 | -16.218 | 16.298 | 1.00 | 54.08 | C |
| ATOM | 873 | O | GLU | A | 134 | 28.319 | -16.114 | 15.094 | 1.00 | 50.66 | O |
| ATOM | 874 | CB | GLU | A | 134 | 26.768 | -17.808 | 16.761 | 1.00 | 58.33 | C |
| ATOM | 875 | CG | GLU | A | 134 | 26.269 | -19.189 | 17.121 | 1.00 | 61.93 | C |
| ATOM | 876 | CD | GLU | A | 134 | 24.955 | -19.558 | 16.436 | 1.00 | 65.28 | C |
| ATOM | 877 | OE1 | GLU | A | 134 | 24.056 | -18.711 | 16.294 | 1.00 | 64.83 | O |
| ATOM | 878 | OE2 | GLU | A | 134 | 24.853 | -20.726 | 16.034 | 1.00 | 68.18 | O |
| ATOM | 879 | N | THR | A | 135 | 28.999 | -15.169 | 16.988 | 1.00 | 52.70 | N |
| ATOM | 880 | CA | THR | A | 135 | 29.366 | -13.953 | 16.291 | 1.00 | 51.61 | C |
| ATOM | 881 | C | THR | A | 135 | 30.896 | -13.856 | 16.192 | 1.00 | 51.35 | C |
| ATOM | 882 | O | THR | A | 135 | 31.549 | -14.721 | 15.580 | 1.00 | 52.93 | O |
| ATOM | 883 | CB | THR | A | 135 | 28.621 | -12.683 | 16.830 | 1.00 | 49.31 | C |
| ATOM | 884 | OG1 | THR | A | 135 | 29.039 | -12.514 | 18.171 | 1.00 | 49.65 | O |
| ATOM | 885 | CG2 | THR | A | 135 | 27.108 | -12.772 | 16.767 | 1.00 | 48.16 | C |
| ATOM | 886 | N | SER | A | 136 | 31.473 | -12.828 | 16.825 | 1.00 | 50.88 | N |
| ATOM | 887 | CA | SER | A | 136 | 32.885 | -12.502 | 16.714 | 1.00 | 49.48 | C |
| ATOM | 888 | C | SER | A | 136 | 33.422 | -12.163 | 18.121 | 1.00 | 47.44 | C |
| ATOM | 889 | O | SER | A | 136 | 32.624 | -12.000 | 19.056 | 1.00 | 46.14 | O |
| ATOM | 890 | CB | SER | A | 136 | 32.966 | -11.306 | 15.767 | 1.00 | 50.00 | C |
| ATOM | 891 | OG | SER | A | 136 | 32.146 | -11.504 | 14.615 | 1.00 | 52.41 | O |
| ATOM | 892 | N | ASP | A | 137 | 34.760 | -12.051 | 18.314 | 1.00 | 44.90 | N |
| ATOM | 893 | CA | ASP | A | 137 | 35.365 | -11.578 | 19.566 | 1.00 | 40.01 | C |
| ATOM | 894 | C | ASP | A | 137 | 35.037 | -10.093 | 19.850 | 1.00 | 36.45 | C |
| ATOM | 895 | O | ASP | A | 137 | 34.105 | -9.570 | 19.228 | 1.00 | 35.34 | O |
| ATOM | 896 | CB | ASP | A | 137 | 36.879 | -11.949 | 19.641 | 1.00 | 40.10 | C |
| ATOM | 897 | CG | ASP | A | 137 | 37.915 | -11.197 | 18.783 | 1.00 | 44.69 | C |
| ATOM | 898 | OD1 | ASP | A | 137 | 37.617 | -10.121 | 18.252 | 1.00 | 46.41 | O |
| ATOM | 899 | OD2 | ASP | A | 137 | 39.056 | -11.661 | 18.648 | 1.00 | 46.87 | O |
| ATOM | 900 | N | CYS | A | 138 | 35.702 | -9.337 | 20.741 | 1.00 | 32.95 | N |
| ATOM | 901 | CA | CYS | A | 138 | 35.263 | -7.982 | 21.014 | 1.00 | 31.28 | C |
| ATOM | 902 | C | CYS | A | 138 | 36.311 | -6.919 | 20.838 | 1.00 | 30.73 | C |
| ATOM | 903 | O | CYS | A | 138 | 36.233 | -5.825 | 21.414 | 1.00 | 31.32 | O |
| ATOM | 904 | CB | CYS | A | 138 | 34.557 | -7.854 | 22.361 | 1.00 | 32.08 | C |

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FIGURE 8A-26

| | | | | | | | | | | |
|------|-----|-----|-------|-----|--------|--------|--------|------|-------|---|
| ATOM | 905 | SG | CYS A | 138 | 32.988 | -8.777 | 22.463 | 1.00 | 37.40 | S |
| ATOM | 906 | N | VAL A | 139 | 37.258 | -7.242 | 19.954 | 1.00 | 30.63 | N |
| ATOM | 907 | CA | VAL A | 139 | 38.333 | -6.318 | 19.599 | 1.00 | 29.74 | C |
| ATOM | 908 | C | VAL A | 139 | 38.151 | -5.898 | 18.168 | 1.00 | 28.81 | C |
| ATOM | 909 | O | VAL A | 139 | 37.830 | -6.734 | 17.342 | 1.00 | 27.95 | O |
| ATOM | 910 | CB | VAL A | 139 | 39.769 | -6.915 | 19.600 | 1.00 | 28.99 | C |
| ATOM | 911 | CG1 | VAL A | 139 | 40.717 | -5.884 | 20.195 | 1.00 | 29.64 | C |
| ATOM | 912 | CG2 | VAL A | 139 | 39.889 | -8.307 | 20.143 | 1.00 | 26.32 | C |
| ATOM | 913 | N | VAL A | 140 | 38.424 | -4.646 | 17.840 | 1.00 | 31.00 | N |
| ATOM | 914 | CA | VAL A | 140 | 38.442 | -4.247 | 16.459 | 1.00 | 34.50 | C |
| ATOM | 915 | C | VAL A | 140 | 39.899 | -4.167 | 16.020 | 1.00 | 36.64 | C |
| ATOM | 916 | O | VAL A | 140 | 40.406 | -5.059 | 15.323 | 1.00 | 39.48 | O |
| ATOM | 917 | CB | VAL A | 140 | 37.758 | -2.914 | 16.217 | 1.00 | 36.55 | C |
| ATOM | 918 | CG1 | VAL A | 140 | 37.417 | -2.900 | 14.747 | 1.00 | 36.42 | C |
| ATOM | 919 | CG2 | VAL A | 140 | 36.594 | -2.569 | 17.119 | 1.00 | 34.81 | C |
| ATOM | 920 | N | SER A | 141 | 40.566 | -3.136 | 16.529 | 1.00 | 37.83 | C |
| ATOM | 921 | CA | SER A | 141 | 41.905 | -2.682 | 16.123 | 1.00 | 41.81 | N |
| ATOM | 922 | C | SER A | 141 | 41.936 | -1.563 | 15.056 | 1.00 | 42.37 | C |
| ATOM | 923 | O | SER A | 141 | 43.035 | -1.174 | 14.685 | 1.00 | 43.60 | O |
| ATOM | 924 | CB | SER A | 141 | 42.986 | -3.811 | 15.889 | 1.00 | 42.08 | C |
| ATOM | 925 | OG | SER A | 141 | 43.175 | -4.693 | 17.008 | 1.00 | 38.01 | O |
| TER | 927 | | SER A | 141 | | | | | | |
| ATOM | 928 | N | ASN B | 11 | 2.666 | 37.382 | 21.946 | 1.00 | 65.93 | N |
| ATOM | 929 | CA | ASN B | 11 | 1.945 | 36.256 | 22.556 | 1.00 | 66.50 | C |
| ATOM | 930 | C | ASN B | 11 | 2.726 | 35.510 | 23.658 | 1.00 | 66.17 | C |
| ATOM | 931 | O | ASN B | 11 | 3.559 | 34.641 | 23.372 | 1.00 | 66.24 | O |
| ATOM | 932 | CB | ASN B | 11 | 1.488 | 35.204 | 21.515 | 1.00 | 66.50 | C |
| ATOM | 933 | N | VAL B | 12 | 2.404 | 35.814 | 24.934 | 1.00 | 65.43 | C |
| ATOM | 934 | CA | VAL B | 12 | 3.197 | 35.450 | 26.131 | 1.00 | 62.92 | N |
| ATOM | 935 | C | VAL B | 12 | 3.195 | 33.985 | 25.631 | 1.00 | 60.27 | C |
| ATOM | 936 | O | VAL B | 12 | 4.143 | 33.547 | 27.294 | 1.00 | 59.00 | O |
| ATOM | 937 | CB | VAL B | 12 | 2.780 | 36.430 | 27.299 | 1.00 | 64.35 | C |
| ATOM | 938 | CG1 | VAL B | 12 | 1.408 | 36.086 | 27.935 | 1.00 | 63.94 | C |
| ATOM | 939 | CG2 | VAL B | 12 | 3.908 | 36.621 | 28.318 | 1.00 | 63.41 | C |
| ATOM | 940 | N | LYS B | 13 | 2.125 | 33.208 | 26.374 | 1.00 | 56.82 | C |
| ATOM | 941 | CA | LYS B | 13 | 2.071 | 31.821 | 26.800 | 1.00 | 51.85 | N |
| ATOM | 942 | C | LYS B | 13 | 3.021 | 31.001 | 25.927 | 1.00 | 48.88 | C |
| ATOM | 943 | O | LYS B | 13 | 3.595 | 30.003 | 26.380 | 1.00 | 49.33 | O |
| ATOM | 944 | CB | LYS B | 13 | 0.640 | 31.283 | 25.675 | 1.00 | 52.25 | C |
| ATOM | 945 | N | ASP B | 14 | 3.258 | 31.456 | 24.684 | 1.00 | 44.12 | C |
| ATOM | 946 | CA | ASP B | 14 | 4.169 | 30.783 | 23.770 | 1.00 | 37.71 | N |
| ATOM | 947 | C | ASP B | 14 | 5.662 | 30.978 | 24.040 | 1.00 | 31.42 | C |
| ATOM | 948 | O | ASP B | 14 | 6.413 | 30.026 | 23.895 | 1.00 | 30.29 | O |
| ATOM | 949 | CB | ASP B | 14 | 3.763 | 31.113 | 22.326 | 1.00 | 40.87 | C |
| ATOM | 950 | CG | ASP B | 14 | 2.497 | 30.409 | 21.803 | 1.00 | 44.08 | C |
| ATOM | 951 | OD1 | ASP B | 14 | 1.832 | 29.636 | 22.531 | 1.00 | 44.87 | O |
| ATOM | 952 | OD2 | ASP B | 14 | 2.192 | 30.662 | 20.631 | 1.00 | 45.27 | O |
| ATOM | 953 | N | VAL B | 15 | 6.165 | 32.130 | 24.468 | 1.00 | 25.72 | C |
| ATOM | 954 | CA | VAL B | 15 | 7.545 | 32.234 | 24.906 | 1.00 | 24.93 | C |
| ATOM | 955 | C | VAL B | 15 | 7.872 | 31.357 | 26.112 | 1.00 | 26.84 | C |
| ATOM | 956 | O | VAL B | 15 | 8.935 | 30.739 | 26.124 | 1.00 | 29.81 | O |
| ATOM | 957 | CB | VAL B | 15 | 7.914 | 33.670 | 25.178 | 1.00 | 22.45 | C |
| ATOM | 958 | CG1 | VAL B | 15 | 9.335 | 33.803 | 25.722 | 1.00 | 18.01 | C |
| ATOM | 959 | CG2 | VAL B | 15 | 7.730 | 34.435 | 23.895 | 1.00 | 21.89 | C |
| ATOM | 960 | N | THR B | 16 | 6.962 | 31.275 | 27.104 | 1.00 | 27.60 | C |
| ATOM | 961 | CA | THR B | 16 | 7.040 | 30.393 | 28.276 | 1.00 | 28.70 | N |
| ATOM | 962 | C | THR B | 16 | 7.191 | 28.905 | 27.903 | 1.00 | 27.24 | C |
| ATOM | 963 | O | THR B | 16 | 8.063 | 28.227 | 28.442 | 1.00 | 29.07 | O |
| ATOM | 964 | CB | THR B | 16 | 5.797 | 30.649 | 29.237 | 1.00 | 30.92 | C |
| ATOM | 965 | OG1 | THR B | 16 | 5.967 | 31.920 | 29.887 | 1.00 | 30.85 | O |

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FIGURE 8A-27

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 966 | CG2 | THR | B | 16 | 5.605 | 29.577 | 30.304 | 1.00 | 29.47 | C |
| ATOM | 967 | N | LYS | B | 17 | 6.385 | 28.387 | 26.979 | 1.00 | 24.02 | N |
| ATOM | 968 | CA | LYS | B | 17 | 6.508 | 27.042 | 26.455 | 1.00 | 25.48 | C |
| ATOM | 969 | C | LYS | B | 17 | 7.776 | 26.845 | 25.607 | 1.00 | 22.72 | C |
| ATOM | 970 | O | LYS | B | 17 | 8.397 | 25.806 | 25.690 | 1.00 | 22.89 | O |
| ATOM | 971 | CB | LYS | B | 17 | 5.235 | 26.851 | 25.662 | 1.00 | 29.47 | C |
| ATOM | 972 | CG | LYS | B | 17 | 5.047 | 25.479 | 25.076 | 1.00 | 36.80 | C |
| ATOM | 973 | CD | LYS | B | 17 | 3.820 | 25.460 | 24.129 | 1.00 | 40.47 | C |
| ATOM | 974 | CE | LYS | B | 17 | 3.432 | 24.008 | 23.742 | 1.00 | 42.23 | C |
| ATOM | 975 | NZ | LYS | B | 17 | 4.518 | 23.260 | 23.099 | 1.00 | 40.28 | N |
| ATOM | 976 | N | LEU | B | 18 | 8.223 | 27.840 | 24.836 | 1.00 | 21.80 | N |
| ATOM | 977 | CA | LEU | B | 18 | 9.489 | 27.797 | 24.148 | 1.00 | 19.84 | N |
| ATOM | 978 | C | LEU | B | 18 | 10.608 | 27.757 | 25.151 | 1.00 | 19.53 | C |
| ATOM | 979 | O | LEU | B | 18 | 11.425 | 26.868 | 24.985 | 1.00 | 22.71 | C |
| ATOM | 980 | CB | LEU | B | 18 | 9.660 | 28.989 | 23.206 | 1.00 | 17.63 | O |
| ATOM | 981 | CG | LEU | B | 18 | 10.954 | 29.148 | 22.479 | 1.00 | 13.25 | C |
| ATOM | 982 | CD1 | LEU | B | 18 | 11.216 | 27.956 | 21.627 | 1.00 | 16.15 | C |
| ATOM | 983 | CD2 | LEU | B | 18 | 10.895 | 30.338 | 21.606 | 1.00 | 13.19 | C |
| ATOM | 984 | N | VAL | B | 19 | 10.670 | 28.606 | 26.187 | 1.00 | 17.49 | N |
| ATOM | 985 | CA | VAL | B | 19 | 11.713 | 28.547 | 27.193 | 1.00 | 15.59 | C |
| ATOM | 986 | C | VAL | B | 19 | 11.708 | 27.199 | 27.912 | 1.00 | 16.76 | C |
| ATOM | 987 | O | VAL | B | 19 | 12.763 | 26.598 | 28.121 | 1.00 | 18.54 | O |
| ATOM | 988 | CB | VAL | B | 19 | 11.587 | 29.741 | 28.170 | 1.00 | 15.79 | C |
| ATOM | 989 | CG1 | VAL | B | 19 | 12.566 | 29.662 | 29.308 | 1.00 | 13.19 | C |
| ATOM | 990 | CG2 | VAL | B | 19 | 11.922 | 31.014 | 27.489 | 1.00 | 12.62 | C |
| ATOM | 991 | N | ALA | B | 20 | 10.533 | 26.655 | 28.232 | 1.00 | 17.26 | N |
| ATOM | 992 | CA | ALA | B | 20 | 10.415 | 25.384 | 28.918 | 1.00 | 17.20 | C |
| ATOM | 993 | C | ALA | B | 20 | 10.866 | 24.235 | 28.075 | 1.00 | 20.20 | C |
| ATOM | 994 | O | ALA | B | 20 | 11.185 | 23.166 | 28.578 | 1.00 | 22.02 | O |
| ATOM | 995 | CB | ALA | B | 20 | 8.972 | 25.064 | 29.185 | 1.00 | 18.25 | C |
| ATOM | 996 | N | ASN | B | 21 | 10.854 | 24.390 | 26.763 | 1.00 | 22.32 | N |
| ATOM | 997 | CA | ASN | B | 21 | 11.373 | 23.351 | 25.920 | 1.00 | 21.93 | C |
| ATOM | 998 | C | ASN | B | 21 | 12.711 | 23.661 | 25.314 | 1.00 | 21.34 | C |
| ATOM | 999 | O | ASN | B | 21 | 13.114 | 22.930 | 24.441 | 1.00 | 23.28 | O |
| ATOM | 1000 | CB | ASN | B | 21 | 10.378 | 23.022 | 24.873 | 1.00 | 26.17 | C |
| ATOM | 1001 | CG | ASN | B | 21 | 9.256 | 22.250 | 25.531 | 1.00 | 31.77 | C |
| ATOM | 1002 | OD1 | ASN | B | 21 | 9.352 | 21.054 | 25.813 | 1.00 | 30.41 | O |
| ATOM | 1003 | ND2 | ASN | B | 21 | 8.168 | 22.955 | 25.820 | 1.00 | 34.22 | N |
| ATOM | 1004 | N | LEU | B | 22 | 13.455 | 24.675 | 25.727 | 1.00 | 20.84 | N |
| ATOM | 1005 | CA | LEU | B | 22 | 14.825 | 24.880 | 25.285 | 1.00 | 18.95 | C |
| ATOM | 1006 | C | LEU | B | 22 | 15.754 | 24.358 | 26.359 | 1.00 | 19.14 | C |
| ATOM | 1007 | O | LEU | B | 22 | 15.428 | 24.560 | 27.526 | 1.00 | 19.71 | O |
| ATOM | 1008 | CB | LEU | B | 22 | 15.097 | 26.380 | 25.022 | 1.00 | 17.41 | C |
| ATOM | 1009 | CG | LEU | B | 22 | 14.510 | 27.035 | 23.750 | 1.00 | 15.79 | C |
| ATOM | 1010 | CD1 | LEU | B | 22 | 14.718 | 28.544 | 23.724 | 1.00 | 13.61 | C |
| ATOM | 1011 | CD2 | LEU | B | 22 | 15.120 | 26.381 | 22.517 | 1.00 | 14.80 | C |
| ATOM | 1012 | N | PRO | B | 23 | 16.903 | 23.701 | 26.091 | 1.00 | 18.35 | N |
| ATOM | 1013 | CA | PRO | B | 23 | 17.831 | 23.260 | 27.130 | 1.00 | 17.51 | C |
| ATOM | 1014 | C | PRO | B | 23 | 18.329 | 24.418 | 28.008 | 1.00 | 17.87 | C |
| ATOM | 1015 | O | PRO | B | 23 | 18.703 | 25.449 | 27.473 | 1.00 | 18.03 | O |
| ATOM | 1016 | CB | PRO | B | 23 | 18.908 | 22.619 | 26.307 | 1.00 | 13.87 | C |
| ATOM | 1017 | CG | PRO | B | 23 | 18.299 | 22.223 | 25.002 | 1.00 | 12.84 | C |
| ATOM | 1018 | CD | PRO | B | 23 | 17.457 | 23.421 | 24.762 | 1.00 | 14.01 | C |
| ATOM | 1019 | N | LYS | B | 24 | 18.327 | 24.340 | 29.347 | 1.00 | 18.87 | N |
| ATOM | 1020 | CA | LYS | B | 24 | 18.756 | 25.441 | 30.226 | 1.00 | 21.96 | C |
| ATOM | 1021 | C | LYS | B | 24 | 20.207 | 25.930 | 30.039 | 1.00 | 21.00 | C |
| ATOM | 1022 | O | LYS | B | 24 | 20.567 | 27.081 | 30.304 | 1.00 | 21.61 | O |
| ATOM | 1023 | CB | LYS | B | 24 | 18.456 | 25.044 | 31.703 | 1.00 | 23.68 | C |
| ATOM | 1024 | CG | LYS | B | 24 | 16.956 | 25.097 | 32.077 | 1.00 | 29.69 | C |
| ATOM | 1025 | CD | LYS | B | 24 | 16.544 | 24.407 | 33.429 | 1.00 | 34.88 | C |

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FIGURE 8A-28

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|----|
| ATOM | 1026 | CE | LYS | B | 24 | 15.010 | 24.526 | 33.777 | 1.00 | 39.45 | C |
| ATOM | 1027 | NZ | LYS | B | 24 | 14.493 | 23.773 | 34.927 | 1.00 | 41.87 | N |
| ATOM | 1028 | N | ASP | B | 25 | 21.040 | 25.044 | 29.503 | 1.00 | 19.08 | N |
| ATOM | 1029 | CA | ASP | B | 25 | 22.440 | 25.350 | 29.263 | 1.00 | 20.79 | C |
| ATOM | 1030 | C | ASP | B | 25 | 22.758 | 25.601 | 27.789 | 1.00 | 19.77 | C |
| ATOM | 1031 | O | ASP | B | 25 | 23.907 | 25.469 | 27.373 | 1.00 | 20.06 | O |
| ATOM | 1032 | CB | ASP | B | 25 | 23.305 | 24.190 | 29.796 | 1.00 | 17.87 | C |
| ATOM | 1033 | CG | ASP | B | 25 | 23.063 | 22.836 | 29.175 | 1.00 | 20.81 | C |
| ATOM | 1034 | OD1 | ASP | B | 25 | 21.975 | 22.598 | 28.651 | 1.00 | 22.64 | C |
| ATOM | 1035 | OD2 | ASP | B | 25 | 23.964 | 21.991 | 29.214 | 1.00 | 24.79 | O |
| ATOM | 1036 | N | TYR | B | 26 | 21.753 | 25.866 | 26.950 | 1.00 | 19.06 | N |
| ATOM | 1037 | CA | TYR | B | 26 | 21.990 | 26.130 | 25.542 | 1.00 | 18.77 | C |
| ATOM | 1038 | C | TYR | B | 26 | 22.027 | 27.652 | 25.358 | 1.00 | 18.82 | C |
| ATOM | 1039 | O | TYR | B | 26 | 21.066 | 28.358 | 25.655 | 1.00 | 19.57 | O |
| ATOM | 1040 | CB | TYR | B | 26 | 20.900 | 25.477 | 24.712 | 1.00 | 16.23 | C |
| ATOM | 1041 | CG | TYR | B | 26 | 21.007 | 25.766 | 23.228 | 1.00 | 19.16 | C |
| ATOM | 1042 | CD1 | TYR | B | 26 | 22.034 | 25.216 | 22.492 | 1.00 | 20.33 | C |
| ATOM | 1043 | CD2 | TYR | B | 26 | 20.097 | 26.629 | 22.632 | 1.00 | 19.21 | C |
| ATOM | 1044 | CE1 | TYR | B | 26 | 22.125 | 25.531 | 21.150 | 1.00 | 19.71 | C |
| ATOM | 1045 | CE2 | TYR | B | 26 | 20.180 | 26.936 | 21.294 | 1.00 | 18.86 | C |
| ATOM | 1046 | CZ | TYR | B | 26 | 21.184 | 26.356 | 20.565 | 1.00 | 21.21 | C |
| ATOM | 1047 | OH | TYR | B | 26 | 21.209 | 26.560 | 19.204 | 1.00 | 23.57 | C |
| HETATM | 1048 | N | MSE | B | 27 | 23.136 | 28.207 | 24.891 | 1.00 | 18.02 | N |
| HETATM | 1049 | CA | MSE | B | 27 | 23.249 | 29.645 | 24.886 | 1.00 | 20.01 | C |
| HETATM | 1050 | C | MSE | B | 27 | 22.894 | 30.253 | 23.553 | 1.00 | 20.43 | C |
| HETATM | 1051 | O | MSE | B | 27 | 23.319 | 29.791 | 22.493 | 1.00 | 22.74 | O |
| HETATM | 1052 | CB | MSE | B | 27 | 24.648 | 30.070 | 25.309 | 1.00 | 21.80 | C |
| HETATM | 1053 | CG | MSE | B | 27 | 25.179 | 29.494 | 26.646 | 1.00 | 24.25 | C |
| HETATM | 1054 | SE | MSE | B | 27 | 24.219 | 29.995 | 28.260 | 1.00 | 30.76 | SE |
| HETATM | 1055 | CE | MSE | B | 27 | 24.936 | 31.691 | 28.317 | 1.00 | 17.91 | C |
| ATOM | 1056 | N | ILE | B | 28 | 22.071 | 31.294 | 23.642 | 1.00 | 21.17 | N |
| ATOM | 1057 | CA | ILE | B | 28 | 21.690 | 32.092 | 22.507 | 1.00 | 20.03 | C |
| ATOM | 1058 | C | ILE | B | 28 | 22.501 | 33.383 | 22.470 | 1.00 | 20.64 | C |
| ATOM | 1059 | O | ILE | B | 28 | 22.545 | 34.162 | 23.403 | 1.00 | 19.83 | O |
| ATOM | 1060 | CB | ILE | B | 28 | 20.168 | 32.289 | 22.522 | 1.00 | 19.56 | C |
| ATOM | 1061 | CG1 | ILE | B | 28 | 19.489 | 30.935 | 22.719 | 1.00 | 14.81 | C |
| ATOM | 1062 | CG2 | ILE | B | 28 | 19.653 | 32.893 | 21.195 | 1.00 | 17.30 | C |
| ATOM | 1063 | CD1 | ILE | B | 28 | 17.993 | 31.054 | 22.978 | 1.00 | 14.38 | C |
| ATOM | 1064 | N | THR | B | 29 | 23.235 | 33.585 | 21.364 | 1.00 | 22.56 | N |
| ATOM | 1065 | CA | THR | B | 29 | 24.048 | 34.777 | 21.117 | 1.00 | 21.92 | C |
| ATOM | 1066 | C | THR | B | 29 | 23.167 | 35.926 | 20.723 | 1.00 | 21.18 | C |
| ATOM | 1067 | O | THR | B | 29 | 22.235 | 35.744 | 19.926 | 1.00 | 24.05 | O |
| ATOM | 1068 | CB | THR | B | 29 | 25.003 | 34.540 | 19.949 | 1.00 | 24.32 | C |
| ATOM | 1069 | OG1 | THR | B | 29 | 25.751 | 33.393 | 20.310 | 1.00 | 26.19 | O |
| ATOM | 1070 | CG2 | THR | B | 29 | 25.901 | 35.743 | 19.657 | 1.00 | 23.45 | C |
| ATOM | 1071 | N | LEU | B | 30 | 23.485 | 37.110 | 21.229 | 1.00 | 19.18 | N |
| ATOM | 1072 | CA | LEU | B | 30 | 22.694 | 38.278 | 20.928 | 1.00 | 19.42 | C |
| ATOM | 1073 | C | LEU | B | 30 | 23.612 | 39.444 | 21.123 | 1.00 | 20.84 | C |
| ATOM | 1074 | O | LEU | B | 30 | 24.251 | 39.604 | 22.155 | 1.00 | 22.59 | O |
| ATOM | 1075 | CB | LEU | B | 30 | 21.486 | 38.458 | 21.822 | 1.00 | 16.57 | C |
| ATOM | 1076 | CG | LEU | B | 30 | 20.712 | 39.739 | 21.692 | 1.00 | 17.65 | C |
| ATOM | 1077 | CD1 | LEU | B | 30 | 19.907 | 39.690 | 20.405 | 1.00 | 15.54 | C |
| ATOM | 1078 | CD2 | LEU | B | 30 | 19.875 | 40.004 | 22.946 | 1.00 | 14.12 | C |
| ATOM | 1079 | N | LYS | B | 31 | 23.641 | 40.271 | 20.085 | 1.00 | 21.41 | N |
| ATOM | 1080 | CA | LYS | B | 31 | 24.340 | 41.533 | 20.142 | 1.00 | 22.33 | C |
| ATOM | 1081 | C | LYS | B | 31 | 23.462 | 42.478 | 20.918 | 1.00 | 21.90 | C |
| ATOM | 1082 | O | LYS | B | 31 | 22.714 | 43.295 | 20.370 | 1.00 | 24.57 | O |
| ATOM | 1083 | CB | LYS | B | 31 | 24.642 | 42.093 | 18.754 | 1.00 | 21.18 | C |
| ATOM | 1084 | CG | LYS | B | 31 | 25.844 | 41.479 | 18.111 | 1.00 | 21.89 | C |
| ATOM | 1085 | CD | LYS | B | 31 | 25.551 | 41.360 | 16.647 | 1.00 | 29.30 | C |

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FIGURE 8A-29

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|----|
| ATOM | 1086 | CE | LYS | B | 31 | 26.741 | 40.957 | 15.808 | 1.00 | 31.29 | C |
| ATOM | 1087 | NZ | LYS | B | 31 | 27.628 | 42.105 | 15.688 | 1.00 | 39.41 | N |
| ATOM | 1088 | N | TYR | B | 32 | 23.572 | 42.299 | 22.227 | 1.00 | 21.32 | C |
| ATOM | 1089 | CA | TYR | B | 32 | 22.800 | 43.101 | 23.138 | 1.00 | 19.60 | N |
| ATOM | 1090 | C | TYR | B | 32 | 23.198 | 44.586 | 22.981 | 1.00 | 19.96 | C |
| ATOM | 1091 | O | TYR | B | 32 | 24.384 | 44.940 | 22.977 | 1.00 | 20.37 | O |
| ATOM | 1092 | CB | TYR | B | 32 | 23.094 | 42.513 | 24.532 | 1.00 | 17.35 | C |
| ATOM | 1093 | CG | TYR | B | 32 | 22.621 | 43.373 | 25.710 | 1.00 | 17.26 | C |
| ATOM | 1094 | CD1 | TYR | B | 32 | 21.298 | 43.297 | 26.107 | 1.00 | 15.20 | C |
| ATOM | 1095 | CD2 | TYR | B | 32 | 23.490 | 44.280 | 26.299 | 1.00 | 14.00 | C |
| ATOM | 1096 | CE1 | TYR | B | 32 | 20.851 | 44.149 | 27.086 | 1.00 | 13.12 | C |
| ATOM | 1097 | CE2 | TYR | B | 32 | 23.013 | 45.166 | 27.227 | 1.00 | 14.39 | C |
| ATOM | 1098 | CZ | TYR | B | 32 | 21.702 | 45.070 | 27.606 | 1.00 | 13.82 | C |
| ATOM | 1099 | OH | TYR | B | 32 | 21.213 | 45.916 | 28.560 | 1.00 | 18.31 | C |
| ATOM | 1100 | N | VAL | B | 33 | 22.179 | 45.455 | 22.873 | 1.00 | 19.13 | N |
| ATOM | 1101 | CA | VAL | B | 33 | 22.376 | 46.889 | 22.818 | 1.00 | 19.34 | C |
| ATOM | 1102 | C | VAL | B | 33 | 22.478 | 47.489 | 24.223 | 1.00 | 22.86 | C |
| ATOM | 1103 | O | VAL | B | 33 | 21.487 | 47.535 | 24.979 | 1.00 | 23.26 | O |
| ATOM | 1104 | CB | VAL | B | 33 | 21.220 | 47.609 | 22.071 | 1.00 | 18.33 | C |
| ATOM | 1105 | CG1 | VAL | B | 33 | 21.607 | 49.014 | 21.732 | 1.00 | 17.72 | C |
| ATOM | 1106 | CG2 | VAL | B | 33 | 20.868 | 46.933 | 20.772 | 1.00 | 18.88 | C |
| ATOM | 1107 | N | PRO | B | 34 | 23.669 | 48.022 | 24.556 | 1.00 | 23.14 | N |
| ATOM | 1108 | CA | PRO | B | 34 | 23.950 | 48.685 | 25.814 | 1.00 | 25.98 | C |
| ATOM | 1109 | C | PRO | B | 34 | 22.991 | 49.844 | 26.052 | 1.00 | 27.87 | C |
| ATOM | 1110 | O | PRO | B | 34 | 22.782 | 50.697 | 25.173 | 1.00 | 28.20 | C |
| ATOM | 1111 | CB | PRO | B | 34 | 25.355 | 49.247 | 25.629 | 1.00 | 24.52 | O |
| ATOM | 1112 | CG | PRO | B | 34 | 25.947 | 48.454 | 24.514 | 1.00 | 23.81 | C |
| ATOM | 1113 | CD | PRO | B | 34 | 24.761 | 48.256 | 23.617 | 1.00 | 23.96 | C |
| ATOM | 1114 | N | GLY | B | 35 | 22.428 | 49.854 | 27.265 | 1.00 | 27.60 | N |
| ATOM | 1115 | CA | GLY | B | 35 | 21.544 | 50.919 | 27.694 | 1.00 | 26.85 | C |
| ATOM | 1116 | C | GLY | B | 35 | 20.103 | 50.509 | 27.809 | 1.00 | 26.95 | C |
| ATOM | 1117 | O | GLY | B | 35 | 19.314 | 51.234 | 28.392 | 1.00 | 27.06 | O |
| HETATM | 1118 | N | MSE | B | 36 | 19.736 | 49.361 | 27.277 | 1.00 | 27.66 | N |
| HETATM | 1119 | CA | MSE | B | 36 | 18.444 | 48.762 | 27.502 | 1.00 | 31.16 | C |
| HETATM | 1120 | C | MSE | B | 36 | 17.873 | 48.948 | 28.920 | 1.00 | 33.96 | C |
| HETATM | 1121 | O | MSE | B | 36 | 16.708 | 49.315 | 29.138 | 1.00 | 34.27 | O |
| HETATM | 1122 | CB | MSE | B | 36 | 18.679 | 47.299 | 27.225 | 1.00 | 34.63 | C |
| HETATM | 1123 | CG | MSE | B | 36 | 17.921 | 46.622 | 26.126 | 1.00 | 37.69 | C |
| HETATM | 1124 | SE | MSE | B | 36 | 16.954 | 45.030 | 26.682 | 1.00 | 48.87 | SE |
| HETATM | 1125 | CE | MSE | B | 36 | 16.692 | 45.161 | 28.580 | 1.00 | 40.22 | C |
| ATOM | 1126 | N | ASP | B | 37 | 18.753 | 48.712 | 29.902 | 1.00 | 35.95 | N |
| ATOM | 1127 | CA | ASP | B | 37 | 18.421 | 48.828 | 31.303 | 1.00 | 37.28 | C |
| ATOM | 1128 | C | ASP | B | 37 | 18.228 | 50.272 | 31.758 | 1.00 | 38.57 | C |
| ATOM | 1129 | O | ASP | B | 37 | 17.189 | 50.545 | 32.368 | 1.00 | 42.23 | O |
| ATOM | 1130 | CB | ASP | B | 37 | 19.407 | 48.058 | 32.203 | 1.00 | 38.21 | C |
| ATOM | 1131 | CG | ASP | B | 37 | 20.907 | 48.280 | 32.005 | 1.00 | 42.18 | C |
| ATOM | 1132 | OD1 | ASP | B | 37 | 21.288 | 49.092 | 31.150 | 1.00 | 44.69 | O |
| ATOM | 1133 | OD2 | ASP | B | 37 | 21.709 | 47.641 | 32.708 | 1.00 | 43.60 | O |
| ATOM | 1134 | N | VAL | B | 38 | 19.111 | 51.237 | 31.458 | 1.00 | 36.46 | N |
| ATOM | 1135 | CA | VAL | B | 38 | 18.974 | 52.585 | 32.008 | 1.00 | 34.42 | C |
| ATOM | 1136 | C | VAL | B | 38 | 18.360 | 53.701 | 31.150 | 1.00 | 35.48 | C |
| ATOM | 1137 | O | VAL | B | 38 | 17.844 | 54.706 | 31.662 | 1.00 | 35.46 | O |
| ATOM | 1138 | CB | VAL | B | 38 | 20.314 | 53.047 | 32.623 | 1.00 | 33.96 | C |
| ATOM | 1139 | CG1 | VAL | B | 38 | 20.656 | 52.110 | 33.757 | 1.00 | 33.39 | C |
| ATOM | 1140 | CG2 | VAL | B | 38 | 21.452 | 53.127 | 31.638 | 1.00 | 30.40 | C |
| ATOM | 1141 | N | LEU | B | 39 | 18.466 | 53.536 | 29.826 | 1.00 | 34.58 | N |
| ATOM | 1142 | CA | LEU | B | 39 | 18.173 | 54.590 | 28.859 | 1.00 | 33.84 | C |
| ATOM | 1143 | C | LEU | B | 39 | 16.770 | 54.521 | 28.304 | 1.00 | 34.39 | C |
| ATOM | 1144 | O | LEU | B | 39 | 16.234 | 53.407 | 28.274 | 1.00 | 37.21 | O |
| ATOM | 1145 | CB | LEU | B | 39 | 19.106 | 54.513 | 27.672 | 1.00 | 31.59 | O |

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FIGURE 8A-30

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 1146 | CG | LEU | B | 39 | 20.516 | 54.934 | 27.836 | 1.00 | 30.49 | C |
| ATOM | 1147 | CD1 | LEU | B | 39 | 21.233 | 54.571 | 26.544 | 1.00 | 30.11 | C |
| ATOM | 1148 | CD2 | LEU | B | 39 | 20.556 | 56.416 | 28.187 | 1.00 | 28.81 | C |
| ATOM | 1149 | N | PRO | B | 40 | 16.124 | 55.613 | 27.821 | 1.00 | 33.22 | C |
| ATOM | 1150 | CA | PRO | B | 40 | 14.743 | 55.564 | 27.336 | 1.00 | 32.18 | N |
| ATOM | 1151 | C | PRO | B | 40 | 14.595 | 54.656 | 26.104 | 1.00 | 31.61 | C |
| ATOM | 1152 | O | PRO | B | 40 | 15.515 | 54.575 | 25.295 | 1.00 | 32.07 | C |
| ATOM | 1153 | CB | PRO | B | 40 | 14.498 | 57.028 | 27.054 | 1.00 | 31.41 | O |
| ATOM | 1154 | CG | PRO | B | 40 | 15.395 | 57.749 | 28.027 | 1.00 | 32.72 | C |
| ATOM | 1155 | CD | PRO | B | 40 | 16.655 | 56.977 | 27.813 | 1.00 | 33.34 | C |
| ATOM | 1156 | N | SER | B | 41 | 13.487 | 53.949 | 25.885 | 1.00 | 31.04 | C |
| ATOM | 1157 | CA | SER | B | 41 | 13.422 | 52.973 | 24.819 | 1.00 | 32.48 | N |
| ATOM | 1158 | C | SER | B | 41 | 13.785 | 53.436 | 23.428 | 1.00 | 32.31 | C |
| ATOM | 1159 | O | SER | B | 41 | 14.301 | 52.651 | 22.638 | 1.00 | 30.86 | O |
| ATOM | 1160 | CB | SER | B | 41 | 12.119 | 52.197 | 24.820 | 1.00 | 34.06 | C |
| ATOM | 1161 | OG | SER | B | 41 | 10.984 | 53.037 | 24.872 | 1.00 | 39.11 | O |
| ATOM | 1162 | N | HIS | B | 42 | 13.622 | 54.747 | 23.191 | 1.00 | 34.63 | N |
| ATOM | 1163 | CA | HIS | B | 42 | 13.911 | 55.363 | 21.888 | 1.00 | 36.02 | C |
| ATOM | 1164 | C | HIS | B | 42 | 15.396 | 55.300 | 21.511 | 1.00 | 36.52 | C |
| ATOM | 1165 | O | HIS | B | 42 | 15.780 | 55.228 | 20.327 | 1.00 | 34.40 | C |
| ATOM | 1166 | CB | HIS | B | 42 | 13.316 | 56.805 | 21.755 | 1.00 | 34.27 | O |
| ATOM | 1167 | CG | HIS | B | 42 | 13.946 | 57.935 | 22.576 | 1.00 | 34.59 | C |
| ATOM | 1168 | ND1 | HIS | B | 42 | 13.588 | 58.408 | 23.772 | 1.00 | 36.14 | N |
| ATOM | 1169 | CD2 | HIS | B | 42 | 15.013 | 58.687 | 22.154 | 1.00 | 32.00 | C |
| ATOM | 1170 | CE1 | HIS | B | 42 | 14.381 | 59.396 | 24.117 | 1.00 | 32.43 | N |
| ATOM | 1171 | NE2 | HIS | B | 42 | 15.227 | 59.539 | 23.124 | 1.00 | 35.02 | C |
| ATOM | 1172 | N | CYS | B | 43 | 16.177 | 55.249 | 22.615 | 1.00 | 35.96 | N |
| ATOM | 1173 | CA | CYS | B | 43 | 17.627 | 55.122 | 22.565 | 1.00 | 35.90 | C |
| ATOM | 1174 | C | CYS | B | 43 | 18.176 | 53.799 | 22.054 | 1.00 | 32.86 | C |
| ATOM | 1175 | O | CYS | B | 43 | 19.347 | 53.782 | 21.649 | 1.00 | 33.40 | C |
| ATOM | 1176 | CB | CYS | B | 43 | 18.339 | 55.448 | 23.910 | 1.00 | 40.38 | O |
| ATOM | 1177 | SG | CYS | B | 43 | 18.099 | 57.127 | 24.542 | 1.00 | 45.68 | C |
| ATOM | 1178 | N | TRP | B | 44 | 17.380 | 52.707 | 22.075 | 1.00 | 29.25 | S |
| ATOM | 1179 | CA | TRP | B | 44 | 17.913 | 51.374 | 21.831 | 1.00 | 25.51 | N |
| ATOM | 1180 | C | TRP | B | 44 | 17.009 | 50.463 | 21.066 | 1.00 | 24.22 | C |
| ATOM | 1181 | O | TRP | B | 44 | 17.544 | 49.594 | 20.406 | 1.00 | 26.02 | C |
| ATOM | 1182 | CB | TRP | B | 44 | 18.375 | 50.661 | 23.113 | 1.00 | 21.99 | O |
| ATOM | 1183 | CG | TRP | B | 44 | 17.351 | 50.644 | 24.234 | 1.00 | 20.34 | C |
| ATOM | 1184 | CD1 | TRP | B | 44 | 17.361 | 51.632 | 25.183 | 1.00 | 18.11 | C |
| ATOM | 1185 | CD2 | TRP | B | 44 | 16.297 | 49.745 | 24.363 | 1.00 | 19.23 | C |
| ATOM | 1186 | NE1 | TRP | B | 44 | 16.293 | 51.390 | 25.908 | 1.00 | 19.12 | N |
| ATOM | 1187 | CE2 | TRP | B | 44 | 15.635 | 50.281 | 25.471 | 1.00 | 18.20 | C |
| ATOM | 1188 | CE3 | TRP | B | 44 | 15.892 | 48.551 | 23.795 | 1.00 | 15.22 | C |
| ATOM | 1189 | CZ2 | TRP | B | 44 | 14.532 | 49.622 | 26.000 | 1.00 | 14.99 | C |
| ATOM | 1190 | CZ3 | TRP | B | 44 | 14.805 | 47.897 | 24.324 | 1.00 | 13.45 | C |
| ATOM | 1191 | CH2 | TRP | B | 44 | 14.130 | 48.434 | 25.405 | 1.00 | 15.50 | C |
| ATOM | 1192 | N | ILE | B | 45 | 15.680 | 50.626 | 21.096 | 1.00 | 24.85 | N |
| ATOM | 1193 | CA | ILE | B | 45 | 14.726 | 49.656 | 20.539 | 1.00 | 25.50 | C |
| ATOM | 1194 | C | ILE | B | 45 | 14.926 | 49.254 | 19.094 | 1.00 | 26.34 | C |
| ATOM | 1195 | O | ILE | B | 45 | 14.724 | 48.086 | 18.762 | 1.00 | 28.11 | O |
| ATOM | 1196 | CB | ILE | B | 45 | 13.231 | 50.055 | 20.773 | 1.00 | 26.28 | O |
| ATOM | 1197 | CG1 | ILE | B | 45 | 12.358 | 48.838 | 20.592 | 1.00 | 24.31 | C |
| ATOM | 1198 | CG2 | ILE | B | 45 | 12.716 | 51.206 | 19.885 | 1.00 | 25.51 | C |
| ATOM | 1199 | CD1 | ILE | B | 45 | 12.688 | 47.633 | 21.486 | 1.00 | 19.41 | C |
| ATOM | 1200 | N | SER | B | 46 | 15.336 | 50.233 | 18.274 | 1.00 | 28.06 | N |
| ATOM | 1201 | CA | SER | B | 46 | 15.623 | 50.071 | 16.851 | 1.00 | 28.67 | C |
| ATOM | 1202 | C | SER | B | 46 | 16.739 | 49.059 | 16.553 | 1.00 | 27.51 | C |
| ATOM | 1203 | O | SER | B | 46 | 16.558 | 48.113 | 15.773 | 1.00 | 26.90 | O |
| ATOM | 1204 | CB | SER | B | 46 | 15.933 | 51.472 | 16.250 | 1.00 | 28.71 | C |
| ATOM | 1205 | OG | SER | B | 46 | 16.259 | 51.414 | 14.871 | 1.00 | 31.35 | O |

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FIGURE 8A-31

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|----|
| ATOM | 1206 | N | GLU | B | 47 | 17.902 | 49.210 | 17.203 | 1.00 | 26.77 | N |
| ATOM | 1207 | CA | GLU | B | 47 | 18.910 | 48.173 | 17.142 | 1.00 | 27.22 | CC |
| ATOM | 1208 | C | GLU | B | 47 | 18.555 | 46.912 | 17.906 | 1.00 | 23.80 | OC |
| ATOM | 1209 | O | GLU | B | 47 | 19.011 | 45.850 | 17.513 | 1.00 | 24.85 | CO |
| ATOM | 1210 | CB | GLU | B | 47 | 20.209 | 48.703 | 17.683 | 1.00 | 30.36 | CC |
| ATOM | 1211 | CG | GLU | B | 47 | 21.460 | 47.909 | 17.269 | 1.00 | 31.64 | CO |
| ATOM | 1212 | CD | GLU | B | 47 | 21.718 | 47.840 | 15.774 | 1.00 | 31.93 | C |
| ATOM | 1213 | OE1 | GLU | B | 47 | 21.267 | 48.726 | 15.034 | 1.00 | 32.82 | OC |
| ATOM | 1214 | OE2 | GLU | B | 47 | 22.391 | 46.892 | 15.366 | 1.00 | 31.60 | CO |
| HETATM | 1215 | N | MSE | B | 48 | 17.739 | 46.958 | 18.958 | 1.00 | 23.65 | O |
| HETATM | 1216 | CA | MSE | B | 48 | 17.401 | 45.755 | 19.709 | 1.00 | 21.94 | N |
| HETATM | 1217 | C | MSE | B | 48 | 16.511 | 44.916 | 18.837 | 1.00 | 22.24 | C |
| HETATM | 1218 | O | MSE | B | 48 | 16.819 | 43.732 | 18.731 | 1.00 | 24.91 | OC |
| HETATM | 1219 | CB | MSE | B | 48 | 16.783 | 46.061 | 21.080 | 1.00 | 22.86 | CC |
| HETATM | 1220 | CG | MSE | B | 48 | 16.875 | 44.981 | 22.173 | 1.00 | 24.51 | CC |
| HETATM | 1221 | SE | MSE | B | 48 | 18.597 | 44.203 | 22.615 | 1.00 | 30.61 | SE |
| HETATM | 1222 | CE | MSE | B | 48 | 17.982 | 42.661 | 21.922 | 1.00 | 26.74 | NC |
| ATOM | 1223 | N | VAL | B | 49 | 15.506 | 45.445 | 18.110 | 1.00 | 21.88 | NC |
| ATOM | 1224 | CA | VAL | B | 49 | 14.661 | 44.597 | 17.276 | 1.00 | 20.25 | C |
| ATOM | 1225 | C | VAL | B | 49 | 15.387 | 43.973 | 16.098 | 1.00 | 20.18 | O |
| ATOM | 1226 | O | VAL | B | 49 | 15.120 | 42.815 | 15.780 | 1.00 | 22.62 | OC |
| ATOM | 1227 | CB | VAL | B | 49 | 13.351 | 45.252 | 16.813 | 1.00 | 23.22 | CC |
| ATOM | 1228 | CG1 | VAL | B | 49 | 12.455 | 45.562 | 17.992 | 1.00 | 24.62 | CC |
| ATOM | 1229 | CG2 | VAL | B | 49 | 13.551 | 46.527 | 16.025 | 1.00 | 23.30 | CC |
| ATOM | 1230 | N | VAL | B | 50 | 16.363 | 44.655 | 15.484 | 1.00 | 19.52 | CC |
| ATOM | 1231 | CA | VAL | B | 50 | 17.179 | 44.087 | 14.408 | 1.00 | 19.02 | NC |
| ATOM | 1232 | C | VAL | B | 50 | 18.005 | 42.916 | 14.897 | 1.00 | 19.73 | CC |
| ATOM | 1233 | O | VAL | B | 50 | 18.091 | 41.872 | 14.232 | 1.00 | 19.76 | OC |
| ATOM | 1234 | CB | VAL | B | 50 | 18.110 | 45.171 | 13.808 | 1.00 | 18.29 | CC |
| ATOM | 1235 | CG1 | VAL | B | 50 | 19.181 | 44.607 | 12.925 | 1.00 | 16.52 | CC |
| ATOM | 1236 | CG2 | VAL | B | 50 | 17.290 | 46.136 | 13.024 | 1.00 | 18.74 | CC |
| ATOM | 1237 | N | GLN | B | 51 | 18.617 | 43.151 | 16.064 | 1.00 | 17.95 | CC |
| ATOM | 1238 | CA | GLN | B | 51 | 19.447 | 42.130 | 16.677 | 1.00 | 18.39 | CC |
| ATOM | 1239 | C | GLN | B | 51 | 18.645 | 40.938 | 17.084 | 1.00 | 16.66 | CC |
| ATOM | 1240 | O | GLN | B | 51 | 19.056 | 39.827 | 16.830 | 1.00 | 18.39 | CC |
| ATOM | 1241 | CB | GLN | B | 51 | 20.264 | 42.655 | 17.851 | 1.00 | 18.87 | CC |
| ATOM | 1242 | CG | GLN | B | 51 | 21.265 | 43.713 | 17.440 | 1.00 | 18.55 | CC |
| ATOM | 1243 | CD | GLN | B | 51 | 22.253 | 43.283 | 16.370 | 1.00 | 23.83 | CC |
| ATOM | 1244 | OE1 | GLN | B | 51 | 22.400 | 42.141 | 15.918 | 1.00 | 23.92 | CC |
| ATOM | 1245 | NE2 | GLN | B | 51 | 23.019 | 44.265 | 15.958 | 1.00 | 27.04 | CC |
| ATOM | 1246 | N | LEU | B | 52 | 17.481 | 41.149 | 17.652 | 1.00 | 16.16 | CC |
| ATOM | 1247 | CA | LEU | B | 52 | 16.615 | 40.053 | 18.010 | 1.00 | 17.66 | CC |
| ATOM | 1248 | C | LEU | B | 52 | 16.106 | 39.302 | 16.810 | 1.00 | 18.23 | CC |
| ATOM | 1249 | O | LEU | B | 52 | 16.012 | 38.080 | 16.844 | 1.00 | 18.09 | CC |
| ATOM | 1250 | CB | LEU | B | 52 | 15.412 | 40.576 | 18.771 | 1.00 | 19.12 | CC |
| ATOM | 1251 | CG | LEU | B | 52 | 15.665 | 40.840 | 20.232 | 1.00 | 20.87 | CC |
| ATOM | 1252 | CD1 | LEU | B | 52 | 14.609 | 41.767 | 20.734 | 1.00 | 20.47 | CC |
| ATOM | 1253 | CD2 | LEU | B | 52 | 15.692 | 39.553 | 21.037 | 1.00 | 21.69 | CC |
| ATOM | 1254 | N | SER | B | 53 | 15.797 | 40.014 | 15.717 | 1.00 | 20.42 | CC |
| ATOM | 1255 | CA | SER | B | 53 | 15.410 | 39.376 | 14.469 | 1.00 | 18.47 | CC |
| ATOM | 1256 | C | SER | B | 53 | 16.491 | 38.428 | 13.973 | 1.00 | 18.27 | CC |
| ATOM | 1257 | O | SER | B | 53 | 16.259 | 37.257 | 13.692 | 1.00 | 17.53 | CC |
| ATOM | 1258 | CB | SER | B | 53 | 15.188 | 40.496 | 13.523 | 1.00 | 21.19 | CC |
| ATOM | 1259 | OG | SER | B | 53 | 14.858 | 39.866 | 12.317 | 1.00 | 22.45 | CC |
| ATOM | 1260 | N | ASP | B | 54 | 17.729 | 38.892 | 13.962 | 1.00 | 21.01 | CC |
| ATOM | 1261 | CA | ASP | B | 54 | 18.811 | 38.060 | 13.483 | 1.00 | 25.15 | CC |
| ATOM | 1262 | C | ASP | B | 54 | 19.040 | 36.841 | 14.339 | 1.00 | 24.43 | CC |
| ATOM | 1263 | O | ASP | B | 54 | 19.279 | 35.764 | 13.782 | 1.00 | 24.72 | CC |
| ATOM | 1264 | CB | ASP | B | 54 | 20.170 | 38.731 | 13.462 | 1.00 | 32.20 | CC |
| ATOM | 1265 | CG | ASP | B | 54 | 20.366 | 40.017 | 12.671 | 1.00 | 44.10 | CC |

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FIGURE 8A-32

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 1266 | OD1 | ASP | B | 54 | 19.508 | 40.411 | 11.838 | 1.00 | 48.06 | O |
| ATOM | 1267 | OD2 | ASP | B | 54 | 21.429 | 40.630 | 12.924 | 1.00 | 50.40 | O |
| ATOM | 1268 | N | SER | B | 55 | 19.025 | 37.009 | 15.674 | 1.00 | 21.94 | N |
| ATOM | 1269 | CA | SER | B | 55 | 19.197 | 35.872 | 16.589 | 1.00 | 21.29 | C |
| ATOM | 1270 | C | SER | B | 55 | 18.036 | 34.884 | 16.516 | 1.00 | 19.86 | O |
| ATOM | 1271 | O | SER | B | 55 | 18.259 | 33.675 | 16.567 | 1.00 | 20.94 | O |
| ATOM | 1272 | CB | SER | B | 55 | 19.356 | 36.295 | 18.052 | 1.00 | 18.68 | O |
| ATOM | 1273 | OG | SER | B | 55 | 20.384 | 37.208 | 18.406 | 1.00 | 18.26 | O |
| ATOM | 1274 | N | LEU | B | 56 | 16.789 | 35.362 | 16.374 | 1.00 | 20.32 | N |
| ATOM | 1275 | CA | LEU | B | 56 | 15.647 | 34.453 | 16.343 | 1.00 | 20.44 | C |
| ATOM | 1276 | C | LEU | B | 56 | 15.628 | 33.735 | 15.025 | 1.00 | 21.16 | O |
| ATOM | 1277 | O | LEU | B | 56 | 15.299 | 32.552 | 14.968 | 1.00 | 20.64 | O |
| ATOM | 1278 | CB | LEU | B | 56 | 14.335 | 35.169 | 16.568 | 1.00 | 19.08 | O |
| ATOM | 1279 | CG | LEU | B | 56 | 13.967 | 35.545 | 17.993 | 1.00 | 19.76 | C |
| ATOM | 1280 | CD1 | LEU | B | 56 | 12.809 | 36.497 | 18.033 | 1.00 | 18.12 | O |
| ATOM | 1281 | CD2 | LEU | B | 56 | 13.621 | 34.308 | 18.773 | 1.00 | 17.63 | C |
| ATOM | 1282 | N | THR | B | 57 | 16.081 | 34.451 | 13.984 | 1.00 | 22.55 | N |
| ATOM | 1283 | CA | THR | B | 57 | 16.144 | 33.901 | 12.624 | 1.00 | 23.77 | C |
| ATOM | 1284 | C | THR | B | 57 | 17.169 | 32.775 | 12.599 | 1.00 | 25.31 | O |
| ATOM | 1285 | O | THR | B | 57 | 16.904 | 31.674 | 12.109 | 1.00 | 28.36 | O |
| ATOM | 1286 | CB | THR | B | 57 | 16.420 | 35.019 | 11.581 | 1.00 | 22.83 | O |
| ATOM | 1287 | OG1 | THR | B | 57 | 15.245 | 35.800 | 11.520 | 1.00 | 20.28 | O |
| ATOM | 1288 | CG2 | THR | B | 57 | 16.608 | 34.496 | 10.209 | 1.00 | 22.98 | O |
| ATOM | 1289 | N | ASP | B | 58 | 18.331 | 32.975 | 13.229 | 1.00 | 27.29 | N |
| ATOM | 1290 | CA | ASP | B | 58 | 19.328 | 31.934 | 13.394 | 1.00 | 25.16 | C |
| ATOM | 1291 | C | ASP | B | 58 | 18.874 | 30.781 | 14.238 | 1.00 | 22.74 | C |
| ATOM | 1292 | O | ASP | B | 58 | 19.128 | 29.640 | 13.909 | 1.00 | 20.50 | O |
| ATOM | 1293 | CB | ASP | B | 58 | 20.510 | 32.549 | 14.059 | 1.00 | 32.90 | O |
| ATOM | 1294 | CG | ASP | B | 58 | 21.367 | 33.343 | 13.098 | 1.00 | 40.22 | O |
| ATOM | 1295 | OD1 | ASP | B | 58 | 21.635 | 32.807 | 11.999 | 1.00 | 47.28 | O |
| ATOM | 1296 | OD2 | ASP | B | 58 | 21.780 | 34.468 | 13.458 | 1.00 | 42.79 | O |
| ATOM | 1297 | N | LEU | B | 59 | 18.174 | 31.090 | 15.328 | 1.00 | 22.88 | N |
| ATOM | 1298 | CA | LEU | B | 59 | 17.597 | 30.066 | 16.166 | 1.00 | 22.01 | C |
| ATOM | 1299 | C | LEU | B | 59 | 16.596 | 29.206 | 15.391 | 1.00 | 22.75 | O |
| ATOM | 1300 | O | LEU | B | 59 | 16.642 | 27.981 | 15.498 | 1.00 | 24.25 | O |
| ATOM | 1301 | CB | LEU | B | 59 | 16.984 | 30.711 | 17.389 | 1.00 | 21.26 | O |
| ATOM | 1302 | CG | LEU | B | 59 | 16.544 | 29.703 | 18.408 | 1.00 | 21.05 | O |
| ATOM | 1303 | CD1 | LEU | B | 59 | 17.733 | 28.955 | 19.020 | 1.00 | 20.13 | O |
| ATOM | 1304 | CD2 | LEU | B | 59 | 15.718 | 30.419 | 19.413 | 1.00 | 20.68 | O |
| ATOM | 1305 | N | LEU | B | 60 | 15.729 | 29.754 | 14.537 | 1.00 | 22.30 | N |
| ATOM | 1306 | CA | LEU | B | 60 | 14.838 | 28.912 | 13.776 | 1.00 | 21.18 | C |
| ATOM | 1307 | C | LEU | B | 60 | 15.559 | 27.884 | 12.897 | 1.00 | 24.69 | O |
| ATOM | 1308 | O | LEU | B | 60 | 15.084 | 26.761 | 12.702 | 1.00 | 27.59 | O |
| ATOM | 1309 | CB | LEU | B | 60 | 13.949 | 29.829 | 12.982 | 1.00 | 20.34 | O |
| ATOM | 1310 | CG | LEU | B | 60 | 12.805 | 29.256 | 12.208 | 1.00 | 15.11 | O |
| ATOM | 1311 | CD1 | LEU | B | 60 | 11.775 | 28.689 | 13.124 | 1.00 | 14.00 | O |
| ATOM | 1312 | CD2 | LEU | B | 60 | 12.216 | 30.351 | 11.405 | 1.00 | 15.62 | O |
| ATOM | 1313 | N | ASP | B | 61 | 16.768 | 28.142 | 12.405 | 1.00 | 28.19 | N |
| ATOM | 1314 | CA | ASP | B | 61 | 17.425 | 27.134 | 11.587 | 1.00 | 31.01 | C |
| ATOM | 1315 | C | ASP | B | 61 | 17.898 | 25.925 | 12.380 | 1.00 | 30.42 | O |
| ATOM | 1316 | O | ASP | B | 61 | 18.293 | 24.903 | 11.836 | 1.00 | 30.78 | O |
| ATOM | 1317 | CB | ASP | B | 61 | 18.486 | 27.766 | 10.638 | 1.00 | 40.38 | O |
| ATOM | 1318 | CG | ASP | B | 61 | 20.011 | 27.910 | 10.913 | 1.00 | 49.60 | O |
| ATOM | 1319 | OD1 | ASP | B | 61 | 20.632 | 27.086 | 11.630 | 1.00 | 52.10 | O |
| ATOM | 1320 | OD2 | ASP | B | 61 | 20.602 | 28.852 | 10.340 | 1.00 | 54.11 | O |
| ATOM | 1321 | N | LYS | B | 62 | 17.841 | 26.023 | 13.706 | 1.00 | 29.72 | N |
| ATOM | 1322 | CA | LYS | B | 62 | 18.282 | 24.972 | 14.586 | 1.00 | 26.53 | C |
| ATOM | 1323 | C | LYS | B | 62 | 17.227 | 23.920 | 14.754 | 1.00 | 26.40 | O |
| ATOM | 1324 | O | LYS | B | 62 | 17.553 | 22.835 | 15.224 | 1.00 | 28.09 | O |
| ATOM | 1325 | CB | LYS | B | 62 | 18.655 | 25.534 | 15.953 | 1.00 | 25.89 | O |

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FIGURE 8A-33

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 1326 | CG | LYS | B | 62 | 19.865 | 26.451 | 15.996 | 1.00 | 24.99 | C |
| ATOM | 1327 | CD | LYS | B | 62 | 21.053 | 25.810 | 15.308 | 1.00 | 26.66 | C |
| ATOM | 1328 | CE | LYS | B | 62 | 22.198 | 26.806 | 15.251 | 1.00 | 28.58 | C |
| ATOM | 1329 | NZ | LYS | B | 62 | 21.868 | 27.957 | 14.431 | 1.00 | 34.52 | N |
| ATOM | 1330 | N | PHE | B | 63 | 15.986 | 24.225 | 14.389 | 1.00 | 26.48 | N |
| ATOM | 1331 | CA | PHE | B | 63 | 14.862 | 23.316 | 14.568 | 1.00 | 29.27 | C |
| ATOM | 1332 | C | PHE | B | 63 | 14.293 | 22.916 | 13.220 | 1.00 | 31.78 | C |
| ATOM | 1333 | O | PHE | B | 63 | 14.573 | 23.581 | 12.227 | 1.00 | 34.39 | C |
| ATOM | 1334 | CB | PHE | B | 63 | 13.744 | 23.920 | 15.427 | 1.00 | 24.13 | O |
| ATOM | 1335 | CG | PHE | B | 63 | 14.261 | 24.236 | 16.809 | 1.00 | 23.83 | C |
| ATOM | 1336 | CD1 | PHE | B | 63 | 14.269 | 23.261 | 17.761 | 1.00 | 20.94 | C |
| ATOM | 1337 | CD2 | PHE | B | 63 | 14.811 | 25.488 | 17.066 | 1.00 | 25.00 | C |
| ATOM | 1338 | CE1 | PHE | B | 63 | 14.872 | 23.535 | 18.964 | 1.00 | 23.54 | C |
| ATOM | 1339 | CE2 | PHE | B | 63 | 15.444 | 25.741 | 18.263 | 1.00 | 22.33 | C |
| ATOM | 1340 | CZ | PHE | B | 63 | 15.467 | 24.752 | 19.211 | 1.00 | 21.46 | C |
| ATOM | 1341 | N | SER | B | 64 | 13.565 | 21.791 | 13.203 | 1.00 | 35.96 | C |
| ATOM | 1342 | CA | SER | B | 64 | 12.847 | 21.251 | 12.047 | 1.00 | 41.24 | N |
| ATOM | 1343 | C | SER | B | 64 | 11.362 | 21.237 | 12.401 | 1.00 | 44.87 | C |
| ATOM | 1344 | O | SER | B | 64 | 11.045 | 21.210 | 13.593 | 1.00 | 45.47 | O |
| ATOM | 1345 | CB | SER | B | 64 | 13.299 | 19.810 | 11.723 | 1.00 | 39.81 | O |
| ATOM | 1346 | OG | SER | B | 64 | 14.690 | 19.659 | 11.441 | 1.00 | 41.15 | O |
| ATOM | 1347 | N | ASN | B | 65 | 10.393 | 21.257 | 11.464 | 1.00 | 50.28 | O |
| ATOM | 1348 | CA | ASN | B | 65 | 8.980 | 21.293 | 11.878 | 1.00 | 53.31 | O |
| ATOM | 1349 | C | ASN | B | 65 | 8.304 | 19.970 | 12.291 | 1.00 | 53.88 | O |
| ATOM | 1350 | O | ASN | B | 65 | 8.619 | 18.877 | 11.815 | 1.00 | 53.27 | O |
| ATOM | 1351 | CB | ASN | B | 65 | 8.137 | 22.121 | 10.899 | 1.00 | 55.21 | O |
| ATOM | 1352 | CG | ASN | B | 65 | 6.847 | 22.674 | 11.525 | 1.00 | 58.28 | O |
| ATOM | 1353 | OD1 | ASN | B | 65 | 5.829 | 22.845 | 10.846 | 1.00 | 62.80 | O |
| ATOM | 1354 | ND2 | ASN | B | 65 | 6.802 | 22.997 | 12.821 | 1.00 | 58.83 | O |
| ATOM | 1355 | N | ILE | B | 66 | 7.402 | 20.111 | 13.274 | 1.00 | 55.78 | N |
| ATOM | 1356 | CA | ILE | B | 66 | 6.604 | 19.028 | 13.857 | 1.00 | 58.20 | N |
| ATOM | 1357 | C | ILE | B | 66 | 5.128 | 19.413 | 13.732 | 1.00 | 59.99 | N |
| ATOM | 1358 | O | ILE | B | 66 | 4.679 | 20.439 | 14.266 | 1.00 | 59.98 | N |
| ATOM | 1359 | CB | ILE | B | 66 | 6.916 | 18.864 | 15.373 | 1.00 | 58.00 | N |
| ATOM | 1360 | CG1 | ILE | B | 66 | 8.393 | 18.635 | 15.673 | 1.00 | 56.77 | N |
| ATOM | 1361 | CG2 | ILE | B | 66 | 6.119 | 17.713 | 15.950 | 1.00 | 58.43 | N |
| ATOM | 1362 | CD1 | ILE | B | 66 | 8.729 | 18.733 | 17.169 | 1.00 | 53.61 | N |
| ATOM | 1363 | N | SER | B | 67 | 4.387 | 18.545 | 13.027 | 1.00 | 62.59 | N |
| ATOM | 1364 | CA | SER | B | 67 | 2.945 | 18.687 | 12.803 | 1.00 | 65.18 | N |
| ATOM | 1365 | C | SER | B | 67 | 2.049 | 18.114 | 13.935 | 1.00 | 66.39 | N |
| ATOM | 1366 | O | SER | B | 67 | 1.110 | 17.339 | 13.725 | 1.00 | 68.18 | N |
| ATOM | 1367 | CB | SER | B | 67 | 2.632 | 18.133 | 11.385 | 1.00 | 65.71 | N |
| ATOM | 1368 | OG | SER | B | 67 | 3.288 | 16.912 | 10.995 | 1.00 | 67.79 | N |
| ATOM | 1369 | N | GLU | B | 68 | 2.307 | 18.549 | 15.184 | 1.00 | 66.59 | N |
| ATOM | 1370 | CA | GLU | B | 68 | 1.793 | 17.929 | 16.415 | 1.00 | 65.52 | N |
| ATOM | 1371 | C | GLU | B | 68 | 0.895 | 18.865 | 17.238 | 1.00 | 66.78 | N |
| ATOM | 1372 | O | GLU | B | 68 | -0.333 | 18.715 | 17.307 | 1.00 | 67.15 | N |
| ATOM | 1373 | CB | GLU | B | 68 | 2.977 | 17.471 | 17.301 | 1.00 | 66.40 | N |
| ATOM | 1374 | CG | GLU | B | 68 | 2.568 | 17.163 | 18.743 | 1.00 | 67.84 | N |
| ATOM | 1375 | CD | GLU | B | 68 | 3.745 | 16.736 | 19.622 | 1.00 | 69.12 | N |
| ATOM | 1376 | OE1 | GLU | B | 68 | 4.931 | 16.661 | 19.119 | 1.00 | 70.46 | N |
| ATOM | 1377 | OE2 | GLU | B | 68 | 3.552 | 16.451 | 20.865 | 1.00 | 71.34 | N |
| ATOM | 1378 | N | GLY | B | 69 | 1.582 | 19.807 | 17.897 | 1.00 | 65.16 | N |
| ATOM | 1379 | CA | GLY | B | 69 | 1.015 | 20.935 | 18.626 | 1.00 | 63.26 | N |
| ATOM | 1380 | C | GLY | B | 69 | 2.019 | 22.049 | 18.382 | 1.00 | 60.63 | N |
| ATOM | 1381 | O | GLY | B | 69 | 2.666 | 22.081 | 17.308 | 1.00 | 60.82 | N |
| ATOM | 1382 | N | LEU | B | 70 | 2.179 | 22.963 | 19.355 | 1.00 | 57.50 | N |
| ATOM | 1383 | CA | LEU | B | 70 | 3.254 | 23.950 | 19.225 | 1.00 | 53.07 | N |
| ATOM | 1384 | C | LEU | B | 70 | 4.610 | 23.233 | 19.244 | 1.00 | 50.38 | N |
| ATOM | 1385 | O | LEU | B | 70 | 4.879 | 22.324 | 20.040 | 1.00 | 53.95 | O |

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FIGURE 8A-34

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 1386 | CB | LEU | B | 70 | 3.243 | 25.033 | 20.295 | 1.00 | 52.74 | C |
| ATOM | 1387 | CG | LEU | B | 70 | 2.243 | 26.184 | 20.332 | 1.00 | 54.01 | C |
| ATOM | 1388 | CD1 | LEU | B | 70 | 2.326 | 26.991 | 19.014 | 1.00 | 54.05 | C |
| ATOM | 1389 | CD2 | LEU | B | 70 | 0.834 | 25.683 | 20.698 | 1.00 | 55.75 | N |
| ATOM | 1390 | N | SER | B | 71 | 5.437 | 23.543 | 18.271 | 1.00 | 43.22 | C |
| ATOM | 1391 | CA | SER | B | 71 | 6.788 | 23.107 | 18.347 | 1.00 | 37.10 | C |
| ATOM | 1392 | C | SER | B | 71 | 7.676 | 24.348 | 18.452 | 1.00 | 35.41 | O |
| ATOM | 1393 | O | SER | B | 71 | 7.223 | 25.469 | 18.195 | 1.00 | 34.32 | C |
| ATOM | 1394 | CB | SER | B | 71 | 7.030 | 22.242 | 17.147 | 1.00 | 36.36 | O |
| ATOM | 1395 | OG | SER | B | 71 | 6.753 | 22.899 | 15.934 | 1.00 | 36.82 | O |
| ATOM | 1396 | N | ASN | B | 72 | 8.946 | 24.206 | 18.876 | 1.00 | 33.26 | N |
| ATOM | 1397 | CA | ASN | B | 72 | 9.888 | 25.327 | 18.974 | 1.00 | 28.70 | C |
| ATOM | 1398 | C | ASN | B | 72 | 10.013 | 26.017 | 17.631 | 1.00 | 25.92 | O |
| ATOM | 1399 | O | ASN | B | 72 | 10.086 | 27.234 | 17.591 | 1.00 | 25.46 | C |
| ATOM | 1400 | CB | ASN | B | 72 | 11.281 | 24.862 | 19.462 | 1.00 | 28.21 | O |
| ATOM | 1401 | CG | ASN | B | 72 | 11.365 | 24.292 | 20.880 | 1.00 | 26.47 | C |
| ATOM | 1402 | OD1 | ASN | B | 72 | 10.592 | 24.638 | 21.764 | 1.00 | 25.38 | O |
| ATOM | 1403 | ND2 | ASN | B | 72 | 12.284 | 23.373 | 21.160 | 1.00 | 26.66 | N |
| ATOM | 1404 | N | TYR | B | 73 | 9.968 | 25.221 | 16.547 | 1.00 | 26.29 | N |
| ATOM | 1405 | CA | TYR | B | 73 | 9.940 | 25.723 | 15.179 | 1.00 | 26.54 | C |
| ATOM | 1406 | C | TYR | B | 73 | 8.760 | 26.639 | 14.993 | 1.00 | 23.80 | O |
| ATOM | 1407 | O | TYR | B | 73 | 8.967 | 27.809 | 14.726 | 1.00 | 27.19 | C |
| ATOM | 1408 | CB | TYR | B | 73 | 9.881 | 24.631 | 14.075 | 1.00 | 28.15 | O |
| ATOM | 1409 | CG | TYR | B | 73 | 10.162 | 25.129 | 12.647 | 1.00 | 28.60 | C |
| ATOM | 1410 | CD1 | TYR | B | 73 | 9.210 | 25.828 | 11.901 | 1.00 | 29.58 | C |
| ATOM | 1411 | CD2 | TYR | B | 73 | 11.426 | 24.929 | 12.122 | 1.00 | 30.26 | C |
| ATOM | 1412 | CE1 | TYR | B | 73 | 9.566 | 26.391 | 10.690 | 1.00 | 29.50 | C |
| ATOM | 1413 | CE2 | TYR | B | 73 | 11.783 | 25.467 | 10.898 | 1.00 | 31.02 | C |
| ATOM | 1414 | CZ | TYR | B | 73 | 10.855 | 26.215 | 10.209 | 1.00 | 32.38 | C |
| ATOM | 1415 | OH | TYR | B | 73 | 11.245 | 26.802 | 9.014 | 1.00 | 36.91 | C |
| ATOM | 1416 | N | SER | B | 74 | 7.535 | 26.185 | 15.145 | 1.00 | 23.20 | O |
| ATOM | 1417 | CA | SER | B | 74 | 6.402 | 27.077 | 15.028 | 1.00 | 24.27 | C |
| ATOM | 1418 | C | SER | B | 74 | 6.449 | 28.270 | 15.935 | 1.00 | 23.26 | O |
| ATOM | 1419 | O | SER | B | 74 | 6.039 | 29.360 | 15.572 | 1.00 | 25.85 | C |
| ATOM | 1420 | CB | SER | B | 74 | 5.156 | 26.342 | 15.357 | 1.00 | 25.27 | O |
| ATOM | 1421 | OG | SER | B | 74 | 5.173 | 25.254 | 14.460 | 1.00 | 32.42 | C |
| ATOM | 1422 | N | ILE | B | 75 | 6.958 | 28.120 | 17.146 | 1.00 | 25.08 | O |
| ATOM | 1423 | CA | ILE | B | 75 | 6.913 | 29.248 | 18.057 | 1.00 | 23.59 | C |
| ATOM | 1424 | C | ILE | B | 75 | 7.908 | 30.294 | 17.620 | 1.00 | 21.89 | O |
| ATOM | 1425 | O | ILE | B | 75 | 7.509 | 31.437 | 17.519 | 1.00 | 21.19 | C |
| ATOM | 1426 | CB | ILE | B | 75 | 7.150 | 28.785 | 19.482 | 1.00 | 23.07 | O |
| ATOM | 1427 | CG1 | ILE | B | 75 | 5.984 | 27.956 | 19.962 | 1.00 | 23.49 | C |
| ATOM | 1428 | CG2 | ILE | B | 75 | 7.272 | 29.985 | 20.397 | 1.00 | 22.81 | C |
| ATOM | 1429 | CD1 | ILE | B | 75 | 6.254 | 27.309 | 21.343 | 1.00 | 21.59 | C |
| ATOM | 1430 | N | ILE | B | 76 | 9.149 | 29.881 | 17.347 | 1.00 | 21.79 | C |
| ATOM | 1431 | CA | ILE | B | 76 | 10.226 | 30.789 | 16.994 | 1.00 | 22.16 | N |
| ATOM | 1432 | C | ILE | B | 76 | 9.830 | 31.465 | 15.705 | 1.00 | 23.36 | C |
| ATOM | 1433 | O | ILE | B | 76 | 9.898 | 32.679 | 15.673 | 1.00 | 26.09 | O |
| ATOM | 1434 | CB | ILE | B | 76 | 11.611 | 30.123 | 16.831 | 1.00 | 21.17 | O |
| ATOM | 1435 | CG1 | ILE | B | 76 | 12.075 | 29.444 | 18.092 | 1.00 | 19.74 | C |
| ATOM | 1436 | CG2 | ILE | B | 76 | 12.661 | 31.169 | 16.489 | 1.00 | 18.62 | C |
| ATOM | 1437 | CD1 | ILE | B | 76 | 13.143 | 28.388 | 17.846 | 1.00 | 17.66 | C |
| ATOM | 1438 | N | ASP | B | 77 | 9.353 | 30.734 | 14.702 | 1.00 | 23.97 | N |
| ATOM | 1439 | CA | ASP | B | 77 | 8.866 | 31.293 | 13.456 | 1.00 | 25.97 | C |
| ATOM | 1440 | C | ASP | B | 77 | 7.856 | 32.411 | 13.657 | 1.00 | 26.70 | O |
| ATOM | 1441 | O | ASP | B | 77 | 8.065 | 33.525 | 13.187 | 1.00 | 28.84 | C |
| ATOM | 1442 | CB | ASP | B | 77 | 8.223 | 30.179 | 12.680 | 1.00 | 28.57 | O |
| ATOM | 1443 | CG | ASP | B | 77 | 8.018 | 30.507 | 11.212 | 1.00 | 32.25 | C |
| ATOM | 1444 | OD1 | ASP | B | 77 | 8.957 | 31.036 | 10.598 | 1.00 | 34.07 | O |
| ATOM | 1445 | OD2 | ASP | B | 77 | 6.927 | 30.224 | 10.704 | 1.00 | 32.50 | C |

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FIGURE 8A-36

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|----|
| ATOM | 1506 | CG | ASP | B | 85 | 4.984 | 42.012 | 11.146 | 1.00 | 36.50 | C |
| ATOM | 1507 | OD1 | ASP | B | 85 | 5.491 | 41.708 | 10.065 | 1.00 | 34.52 | CO |
| ATOM | 1508 | OD2 | ASP | B | 85 | 3.945 | 41.485 | 11.574 | 1.00 | 37.36 | N |
| ATOM | 1509 | N | LEU | B | 86 | 8.151 | 44.567 | 13.473 | 1.00 | 31.94 | CC |
| ATOM | 1510 | CA | LEU | B | 86 | 8.695 | 45.686 | 14.241 | 1.00 | 29.00 | CO |
| ATOM | 1511 | C | LEU | B | 86 | 9.945 | 46.335 | 13.646 | 1.00 | 27.01 | C |
| ATOM | 1512 | O | LEU | B | 86 | 10.158 | 47.536 | 13.788 | 1.00 | 25.07 | CO |
| ATOM | 1513 | CB | LEU | B | 86 | 8.888 | 45.242 | 15.703 | 1.00 | 29.72 | C |
| ATOM | 1514 | CG | LEU | B | 86 | 7.630 | 44.973 | 16.544 | 1.00 | 29.69 | CC |
| ATOM | 1515 | CD1 | LEU | B | 86 | 7.934 | 44.246 | 17.825 | 1.00 | 29.68 | C |
| ATOM | 1516 | CD2 | LEU | B | 86 | 6.938 | 46.265 | 16.914 | 1.00 | 29.39 | CC |
| ATOM | 1517 | N | VAL | B | 87 | 10.774 | 45.550 | 12.962 | 1.00 | 26.28 | C |
| ATOM | 1518 | CA | VAL | B | 87 | 11.895 | 46.068 | 12.214 | 1.00 | 29.27 | NC |
| ATOM | 1519 | C | VAL | B | 87 | 11.333 | 47.009 | 11.163 | 1.00 | 32.65 | CC |
| ATOM | 1520 | O | VAL | B | 87 | 11.721 | 48.175 | 11.164 | 1.00 | 35.43 | C |
| ATOM | 1521 | CB | VAL | B | 87 | 12.725 | 44.966 | 11.523 | 1.00 | 28.93 | CO |
| ATOM | 1522 | CG1 | VAL | B | 87 | 13.789 | 45.570 | 10.630 | 1.00 | 25.59 | CC |
| ATOM | 1523 | CG2 | VAL | B | 87 | 13.417 | 44.036 | 12.521 | 1.00 | 30.50 | C |
| ATOM | 1524 | N | GLU | B | 88 | 10.392 | 46.534 | 10.325 | 1.00 | 34.28 | NC |
| ATOM | 1525 | CA | GLU | B | 88 | 9.820 | 47.291 | 9.217 | 1.00 | 34.18 | C |
| ATOM | 1526 | C | GLU | B | 88 | 9.201 | 48.582 | 9.702 | 1.00 | 34.90 | CC |
| ATOM | 1527 | O | GLU | B | 88 | 9.505 | 49.640 | 9.178 | 1.00 | 35.08 | C |
| ATOM | 1528 | CB | GLU | B | 88 | 8.789 | 46.446 | 8.468 | 1.00 | 34.62 | CC |
| ATOM | 1529 | CG | GLU | B | 88 | 9.361 | 45.233 | 7.725 | 1.00 | 35.13 | C |
| ATOM | 1530 | CD | GLU | B | 88 | 8.360 | 44.218 | 7.145 | 1.00 | 37.81 | CC |
| ATOM | 1531 | OE1 | GLU | B | 88 | 7.241 | 44.088 | 7.653 | 1.00 | 39.42 | CO |
| ATOM | 1532 | OE2 | GLU | B | 88 | 8.696 | 43.539 | 6.176 | 1.00 | 38.59 | CO |
| ATOM | 1533 | N | CYS | B | 89 | 8.402 | 48.520 | 10.754 | 1.00 | 37.74 | NC |
| ATOM | 1534 | CA | CYS | B | 89 | 7.803 | 49.680 | 11.378 | 1.00 | 41.43 | CC |
| ATOM | 1535 | C | CYS | B | 89 | 8.798 | 50.685 | 11.934 | 1.00 | 43.62 | C |
| ATOM | 1536 | O | CYS | B | 89 | 8.578 | 51.896 | 11.896 | 1.00 | 44.63 | CC |
| ATOM | 1537 | CB | CYS | B | 89 | 6.875 | 49.166 | 12.472 | 1.00 | 43.51 | C |
| ATOM | 1538 | SG | CYS | B | 89 | 6.538 | 50.326 | 13.821 | 1.00 | 52.54 | CS |
| ATOM | 1539 | N | VAL | B | 90 | 9.907 | 50.205 | 12.473 | 1.00 | 45.45 | N |
| ATOM | 1540 | CA | VAL | B | 90 | 10.919 | 51.096 | 13.007 | 1.00 | 48.36 | CC |
| ATOM | 1541 | C | VAL | B | 90 | 11.787 | 51.723 | 11.909 | 1.00 | 49.57 | C |
| ATOM | 1542 | O | VAL | B | 90 | 12.399 | 52.768 | 12.121 | 1.00 | 50.61 | CO |
| ATOM | 1543 | CB | VAL | B | 90 | 11.681 | 50.331 | 14.107 | 1.00 | 48.77 | C |
| ATOM | 1544 | CG1 | VAL | B | 90 | 12.903 | 51.039 | 14.582 | 1.00 | 51.24 | CC |
| ATOM | 1545 | CG2 | VAL | B | 90 | 10.793 | 50.256 | 15.316 | 1.00 | 48.76 | C |
| ATOM | 1546 | N | LYS | B | 91 | 11.834 | 51.181 | 10.695 | 1.00 | 50.84 | NC |
| ATOM | 1547 | CA | LYS | B | 91 | 12.492 | 51.870 | 9.600 | 1.00 | 52.46 | C |
| ATOM | 1548 | C | LYS | B | 91 | 11.615 | 52.881 | 8.847 | 1.00 | 53.71 | CC |
| ATOM | 1549 | O | LYS | B | 91 | 12.139 | 53.730 | 8.127 | 1.00 | 52.07 | C |
| ATOM | 1550 | CB | LYS | B | 91 | 13.135 | 50.840 | 8.721 | 1.00 | 54.00 | CC |
| ATOM | 1551 | CG | LYS | B | 91 | 14.290 | 50.209 | 9.508 | 1.00 | 59.12 | C |
| ATOM | 1552 | CD | LYS | B | 91 | 14.955 | 49.089 | 8.690 | 1.00 | 63.16 | CC |
| ATOM | 1553 | CE | LYS | B | 91 | 16.176 | 48.420 | 9.367 | 1.00 | 66.55 | C |
| ATOM | 1554 | NZ | LYS | B | 91 | 16.631 | 47.252 | 8.605 | 1.00 | 68.43 | CC |
| ATOM | 1555 | N | GLU | B | 92 | 10.283 | 52.858 | 9.066 | 1.00 | 56.63 | N |
| ATOM | 1556 | CA | GLU | B | 92 | 9.333 | 53.861 | 8.565 | 1.00 | 59.16 | CC |
| ATOM | 1557 | C | GLU | B | 92 | 9.366 | 55.130 | 9.381 | 1.00 | 60.82 | C |
| ATOM | 1558 | O | GLU | B | 92 | 9.635 | 56.189 | 8.802 | 1.00 | 61.59 | CC |
| ATOM | 1559 | CB | GLU | B | 92 | 7.852 | 53.434 | 8.599 | 1.00 | 60.60 | C |
| ATOM | 1560 | CG | GLU | B | 92 | 7.388 | 52.228 | 7.784 | 1.00 | 63.20 | CC |
| ATOM | 1561 | CD | GLU | B | 92 | 7.621 | 52.275 | 6.273 | 1.00 | 66.00 | C |
| ATOM | 1562 | OE1 | GLU | B | 92 | 7.843 | 53.369 | 5.709 | 1.00 | 65.65 | CC |
| ATOM | 1563 | OE2 | GLU | B | 92 | 7.564 | 51.187 | 5.667 | 1.00 | 67.41 | C |
| ATOM | 1564 | N | ASN | B | 93 | 9.061 | 54.977 | 10.598 | 1.00 | 62.57 | CO |
| ATOM | 1565 | CA | ASN | B | 93 | 9.063 | 56.041 | 11.714 | 1.00 | 64.84 | CO |

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FIGURE 8A-37

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|-----|
| ATOM | 1566 | C | ASN | B | 93 | 10.247 | 56.971 | 11.593 | 1.00 | 65.46 | C |
| ATOM | 1567 | O | ASN | B | 93 | 11.368 | 56.721 | 12.018 | 1.00 | 65.03 | O |
| ATOM | 1568 | CB | ASN | B | 93 | 9.069 | 55.511 | 13.153 | 1.00 | 63.55 | C |
| ATOM | 1569 | N | SER | B | 94 | 9.868 | 58.041 | 10.904 | 1.00 | 68.52 | N |
| ATOM | 1570 | CA | SER | B | 94 | 10.773 | 58.985 | 10.254 | 1.00 | 70.87 | C |
| ATOM | 1571 | C | SER | B | 94 | 11.391 | 60.076 | 11.141 | 1.00 | 71.17 | C |
| ATOM | 1572 | O | SER | B | 94 | 12.292 | 60.821 | 10.689 | 1.00 | 72.46 | C |
| ATOM | 1573 | CB | SER | B | 94 | 10.028 | 59.573 | 9.039 | 1.00 | 71.38 | O |
| ATOM | 1574 | OG | SER | B | 94 | 8.711 | 60.001 | 9.407 | 1.00 | 73.36 | O |
| ATOM | 1575 | N | SER | B | 95 | 10.923 | 60.135 | 12.415 | 1.00 | 68.97 | CON |
| ATOM | 1576 | CA | SER | B | 95 | 11.564 | 60.953 | 13.424 | 1.00 | 68.06 | C |
| ATOM | 1577 | C | SER | B | 95 | 13.040 | 60.572 | 13.473 | 1.00 | 67.28 | C |
| ATOM | 1578 | O | SER | B | 95 | 13.457 | 59.458 | 13.839 | 1.00 | 64.89 | O |
| ATOM | 1579 | CB | SER | B | 95 | 10.932 | 60.795 | 14.794 | 1.00 | 68.06 | O |
| ATOM | 1580 | OG | SER | B | 95 | 11.441 | 61.800 | 15.670 | 1.00 | 69.36 | O |
| ATOM | 1581 | N | LYS | B | 96 | 13.755 | 61.565 | 12.916 | 1.00 | 66.92 | CON |
| ATOM | 1582 | CA | LYS | B | 96 | 15.199 | 61.518 | 12.771 | 1.00 | 67.27 | C |
| ATOM | 1583 | C | LYS | B | 96 | 15.848 | 60.974 | 14.056 | 1.00 | 66.10 | C |
| ATOM | 1584 | O | LYS | B | 96 | 16.615 | 59.996 | 14.014 | 1.00 | 64.46 | C |
| ATOM | 1585 | CB | LYS | B | 96 | 15.699 | 62.948 | 12.478 | 1.00 | 67.07 | O |
| ATOM | 1586 | N | ASP | B | 97 | 15.289 | 61.560 | 15.147 | 1.00 | 64.54 | C |
| ATOM | 1587 | CA | ASP | B | 97 | 15.657 | 61.369 | 16.562 | 1.00 | 62.82 | N |
| ATOM | 1588 | C | ASP | B | 97 | 15.739 | 59.968 | 17.239 | 1.00 | 60.00 | C |
| ATOM | 1589 | O | ASP | B | 97 | 16.792 | 59.674 | 17.852 | 1.00 | 59.90 | C |
| ATOM | 1590 | CB | ASP | B | 97 | 14.689 | 62.230 | 17.394 | 1.00 | 63.85 | O |
| ATOM | 1591 | N | LEU | B | 98 | 14.638 | 59.137 | 17.174 | 1.00 | 53.67 | C |
| ATOM | 1592 | CA | LEU | B | 98 | 14.641 | 57.690 | 17.447 | 1.00 | 44.35 | N |
| ATOM | 1593 | C | LEU | B | 98 | 15.837 | 57.135 | 16.728 | 1.00 | 40.32 | C |
| ATOM | 1594 | O | LEU | B | 98 | 15.868 | 57.109 | 15.497 | 1.00 | 40.10 | C |
| ATOM | 1595 | CB | LEU | B | 98 | 13.389 | 56.996 | 16.916 | 1.00 | 41.21 | O |
| ATOM | 1596 | CG | LEU | B | 98 | 13.251 | 55.479 | 17.095 | 1.00 | 40.48 | C |
| ATOM | 1597 | CD1 | LEU | B | 98 | 11.904 | 55.030 | 17.695 | 1.00 | 39.61 | C |
| ATOM | 1598 | CD2 | LEU | B | 98 | 13.519 | 54.787 | 15.784 | 1.00 | 37.90 | C |
| ATOM | 1599 | N | LYS | B | 99 | 16.815 | 56.840 | 17.593 | 1.00 | 36.84 | C |
| ATOM | 1600 | CA | LYS | B | 99 | 18.171 | 56.457 | 17.229 | 1.00 | 35.08 | N |
| ATOM | 1601 | C | LYS | B | 99 | 18.141 | 55.218 | 16.365 | 1.00 | 34.40 | C |
| ATOM | 1602 | O | LYS | B | 99 | 17.600 | 54.164 | 16.712 | 1.00 | 34.91 | O |
| ATOM | 1603 | CB | LYS | B | 99 | 19.028 | 56.193 | 18.485 | 1.00 | 35.16 | C |
| ATOM | 1604 | CG | LYS | B | 99 | 20.550 | 56.058 | 18.286 | 1.00 | 37.24 | C |
| ATOM | 1605 | CD | LYS | B | 99 | 21.314 | 55.641 | 19.556 | 1.00 | 36.33 | C |
| ATOM | 1606 | CE | LYS | B | 99 | 22.817 | 55.994 | 19.594 | 1.00 | 38.98 | C |
| ATOM | 1607 | NZ | LYS | B | 99 | 23.617 | 55.657 | 18.428 | 1.00 | 38.67 | C |
| ATOM | 1608 | N | LYS | B | 100 | 18.689 | 55.387 | 15.174 | 1.00 | 34.28 | N |
| ATOM | 1609 | CA | LYS | B | 100 | 18.726 | 54.285 | 14.232 | 1.00 | 34.35 | C |
| ATOM | 1610 | C | LYS | B | 100 | 20.147 | 53.964 | 13.811 | 1.00 | 31.26 | C |
| ATOM | 1611 | O | LYS | B | 100 | 20.368 | 52.917 | 13.224 | 1.00 | 32.09 | O |
| ATOM | 1612 | CB | LYS | B | 100 | 17.832 | 54.592 | 13.044 | 1.00 | 36.01 | C |
| ATOM | 1613 | CG | LYS | B | 100 | 16.335 | 54.635 | 13.349 | 1.00 | 38.72 | C |
| ATOM | 1614 | CD | LYS | B | 100 | 15.782 | 55.851 | 12.617 | 1.00 | 43.22 | C |
| ATOM | 1615 | CE | LYS | B | 100 | 14.290 | 55.723 | 12.370 | 1.00 | 43.50 | C |
| ATOM | 1616 | NZ | LYS | B | 100 | 13.982 | 55.990 | 10.969 | 1.00 | 43.57 | C |
| ATOM | 1617 | N | SER | B | 101 | 21.120 | 54.814 | 14.159 | 1.00 | 29.00 | N |
| ATOM | 1618 | CA | SER | B | 101 | 22.529 | 54.614 | 13.871 | 1.00 | 28.55 | C |
| ATOM | 1619 | C | SER | B | 101 | 23.351 | 54.047 | 15.032 | 1.00 | 28.24 | C |
| ATOM | 1620 | O | SER | B | 101 | 23.732 | 54.783 | 15.943 | 1.00 | 31.98 | C |
| ATOM | 1621 | CB | SER | B | 101 | 23.049 | 55.977 | 13.473 | 1.00 | 27.88 | C |
| ATOM | 1622 | OG | SER | B | 101 | 24.459 | 55.979 | 13.457 | 1.00 | 27.09 | C |
| ATOM | 1623 | N | PHE | B | 102 | 23.680 | 52.766 | 15.077 | 1.00 | 27.56 | C |
| ATOM | 1624 | CA | PHE | B | 102 | 24.364 | 52.184 | 16.230 | 1.00 | 27.12 | N |
| ATOM | 1625 | C | PHE | B | 102 | 25.620 | 51.495 | 15.755 | 1.00 | 28.99 | C |

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FIGURE 8A-38

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1626 | O | PHE | B | 102 | 25.613 | 51.001 | 14.627 | 1.00 | 28.31 | O |
| ATOM | 1627 | CB | PHE | B | 102 | 23.538 | 51.127 | 16.945 | 1.00 | 22.35 | C |
| ATOM | 1628 | CG | PHE | B | 102 | 22.247 | 51.672 | 17.462 | 1.00 | 20.73 | C |
| ATOM | 1629 | CD1 | PHE | B | 102 | 21.206 | 51.877 | 16.608 | 1.00 | 22.70 | C |
| ATOM | 1630 | CD2 | PHE | B | 102 | 22.105 | 51.932 | 18.801 | 1.00 | 24.01 | C |
| ATOM | 1631 | CE1 | PHE | B | 102 | 20.007 | 52.325 | 17.098 | 1.00 | 23.86 | C |
| ATOM | 1632 | CE2 | PHE | B | 102 | 20.892 | 52.343 | 19.295 | 1.00 | 23.54 | C |
| ATOM | 1633 | CZ | PHE | B | 102 | 19.837 | 52.536 | 18.435 | 1.00 | 23.17 | C |
| ATOM | 1634 | N | LYS | B | 103 | 26.691 | 51.459 | 16.575 | 1.00 | 30.21 | C |
| ATOM | 1635 | CA | LYS | B | 103 | 27.823 | 50.595 | 16.284 | 1.00 | 30.86 | N |
| ATOM | 1636 | C | LYS | B | 103 | 27.374 | 49.171 | 16.550 | 1.00 | 32.14 | C |
| ATOM | 1637 | O | LYS | B | 103 | 26.583 | 48.957 | 17.472 | 1.00 | 33.74 | C |
| ATOM | 1638 | CB | LYS | B | 103 | 28.965 | 50.952 | 17.200 | 1.00 | 32.77 | O |
| ATOM | 1639 | N | SER | B | 104 | 27.788 | 48.202 | 15.720 | 1.00 | 32.95 | C |
| ATOM | 1640 | CA | SER | B | 104 | 27.284 | 46.825 | 15.805 | 1.00 | 33.85 | N |
| ATOM | 1641 | C | SER | B | 104 | 27.695 | 46.249 | 17.145 | 1.00 | 31.14 | C |
| ATOM | 1642 | O | SER | B | 104 | 28.891 | 46.121 | 17.418 | 1.00 | 32.16 | C |
| ATOM | 1643 | CB | SER | B | 104 | 27.812 | 45.908 | 14.692 | 1.00 | 36.29 | O |
| ATOM | 1644 | OG | SER | B | 104 | 28.690 | 46.589 | 13.784 | 1.00 | 44.97 | C |
| ATOM | 1645 | N | PRO | B | 105 | 26.737 | 45.950 | 18.023 | 1.00 | 28.62 | O |
| ATOM | 1646 | CA | PRO | B | 105 | 27.026 | 45.601 | 19.393 | 1.00 | 27.39 | N |
| ATOM | 1647 | C | PRO | B | 105 | 27.816 | 44.315 | 19.472 | 1.00 | 26.85 | C |
| ATOM | 1648 | O | PRO | B | 105 | 27.947 | 43.532 | 18.527 | 1.00 | 29.04 | C |
| ATOM | 1649 | CB | PRO | B | 105 | 25.668 | 45.476 | 19.982 | 1.00 | 26.67 | O |
| ATOM | 1650 | CG | PRO | B | 105 | 24.803 | 46.313 | 19.104 | 1.00 | 26.85 | C |
| ATOM | 1651 | CD | PRO | B | 105 | 25.308 | 45.910 | 17.747 | 1.00 | 26.48 | C |
| ATOM | 1652 | N | GLU | B | 106 | 28.426 | 44.160 | 20.628 | 1.00 | 27.12 | N |
| ATOM | 1653 | CA | GLU | B | 106 | 29.240 | 42.982 | 20.897 | 1.00 | 27.97 | C |
| ATOM | 1654 | C | GLU | B | 106 | 28.299 | 41.806 | 21.172 | 1.00 | 25.13 | C |
| ATOM | 1655 | O | GLU | B | 106 | 27.294 | 41.966 | 21.870 | 1.00 | 21.99 | C |
| ATOM | 1656 | CB | GLU | B | 106 | 30.140 | 43.258 | 22.105 | 1.00 | 30.05 | O |
| ATOM | 1657 | CG | GLU | B | 106 | 31.418 | 42.451 | 22.220 | 1.00 | 35.47 | C |
| ATOM | 1658 | CD | GLU | B | 106 | 32.045 | 42.483 | 23.613 | 1.00 | 40.01 | C |
| ATOM | 1659 | OE1 | GLU | B | 106 | 32.162 | 43.570 | 24.198 | 1.00 | 41.10 | C |
| ATOM | 1660 | OE2 | GLU | B | 106 | 32.431 | 41.409 | 24.102 | 1.00 | 42.35 | O |
| ATOM | 1661 | N | PRO | B | 107 | 28.564 | 40.640 | 20.578 | 1.00 | 23.74 | O |
| ATOM | 1662 | CA | PRO | B | 107 | 27.806 | 39.423 | 20.817 | 1.00 | 24.07 | N |
| ATOM | 1663 | C | PRO | B | 107 | 27.906 | 38.967 | 22.264 | 1.00 | 22.95 | C |
| ATOM | 1664 | O | PRO | B | 107 | 28.989 | 38.920 | 22.832 | 1.00 | 24.47 | C |
| ATOM | 1665 | CB | PRO | B | 107 | 28.437 | 38.439 | 19.837 | 1.00 | 24.75 | O |
| ATOM | 1666 | CG | PRO | B | 107 | 28.949 | 39.309 | 18.715 | 1.00 | 25.17 | C |
| ATOM | 1667 | CD | PRO | B | 107 | 29.556 | 40.448 | 19.512 | 1.00 | 24.46 | C |
| ATOM | 1668 | N | ARG | B | 108 | 26.765 | 38.677 | 22.884 | 1.00 | 22.39 | C |
| ATOM | 1669 | CA | ARG | B | 108 | 26.684 | 38.164 | 24.239 | 1.00 | 20.57 | N |
| ATOM | 1670 | C | ARG | B | 108 | 25.904 | 36.865 | 24.227 | 1.00 | 17.43 | C |
| ATOM | 1671 | O | ARG | B | 108 | 24.954 | 36.685 | 23.488 | 1.00 | 17.22 | C |
| ATOM | 1672 | CB | ARG | B | 108 | 26.064 | 39.155 | 25.256 | 1.00 | 20.10 | C |
| ATOM | 1673 | CG | ARG | B | 108 | 27.007 | 40.157 | 25.848 | 1.00 | 21.68 | C |
| ATOM | 1674 | CD | ARG | B | 108 | 26.321 | 41.144 | 26.778 | 1.00 | 25.69 | C |
| ATOM | 1675 | NE | ARG | B | 108 | 25.859 | 40.576 | 28.047 | 1.00 | 27.65 | N |
| ATOM | 1676 | CZ | ARG | B | 108 | 25.517 | 41.345 | 29.084 | 1.00 | 26.15 | C |
| ATOM | 1677 | NH1 | ARG | B | 108 | 25.637 | 42.653 | 29.004 | 1.00 | 26.98 | C |
| ATOM | 1678 | NH2 | ARG | B | 108 | 25.031 | 40.819 | 30.217 | 1.00 | 27.28 | N |
| ATOM | 1679 | N | LEU | B | 109 | 26.320 | 35.964 | 25.078 | 1.00 | 16.44 | N |
| ATOM | 1680 | CA | LEU | B | 109 | 25.649 | 34.700 | 25.242 | 1.00 | 19.58 | C |
| ATOM | 1681 | C | LEU | B | 109 | 24.667 | 34.827 | 26.384 | 1.00 | 19.57 | C |
| ATOM | 1682 | O | LEU | B | 109 | 24.963 | 35.423 | 27.418 | 1.00 | 21.90 | C |
| ATOM | 1683 | CB | LEU | B | 109 | 26.626 | 33.555 | 25.533 | 1.00 | 18.89 | C |
| ATOM | 1684 | CG | LEU | B | 109 | 27.661 | 33.129 | 24.491 | 1.00 | 20.14 | C |
| ATOM | 1685 | CD1 | LEU | B | 109 | 28.673 | 32.188 | 25.119 | 1.00 | 18.71 | C |

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FIGURE 8A-39

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1686 | CD2 | LEU | B | 109 | 26.985 | 32.436 | 23.316 | 1.00 | 22.74 | C |
| ATOM | 1687 | N | PHE | B | 110 | 23.477 | 34.293 | 26.119 | 1.00 | 19.30 | N |
| ATOM | 1688 | CA | PHE | B | 110 | 22.372 | 34.322 | 27.050 | 1.00 | 18.85 | C |
| ATOM | 1689 | C | PHE | B | 110 | 21.748 | 32.939 | 27.188 | 1.00 | 19.38 | C |
| ATOM | 1690 | O | PHE | B | 110 | 21.676 | 32.205 | 26.207 | 1.00 | 18.43 | C |
| ATOM | 1691 | CB | PHE | B | 110 | 21.312 | 35.298 | 26.553 | 1.00 | 17.38 | O |
| ATOM | 1692 | CG | PHE | B | 110 | 21.743 | 36.756 | 26.567 | 1.00 | 19.20 | C |
| ATOM | 1693 | CD1 | PHE | B | 110 | 21.733 | 37.487 | 27.744 | 1.00 | 20.10 | C |
| ATOM | 1694 | CD2 | PHE | B | 110 | 22.198 | 37.350 | 25.408 | 1.00 | 19.07 | C |
| ATOM | 1695 | CE1 | PHE | B | 110 | 22.211 | 38.788 | 27.755 | 1.00 | 19.86 | C |
| ATOM | 1696 | CE2 | PHE | B | 110 | 22.643 | 38.650 | 25.436 | 1.00 | 15.79 | C |
| ATOM | 1697 | CZ | PHE | B | 110 | 22.659 | 39.367 | 26.596 | 1.00 | 17.86 | C |
| ATOM | 1698 | N | THR | B | 111 | 21.246 | 32.547 | 28.376 | 1.00 | 18.40 | N |
| ATOM | 1699 | CA | THR | B | 111 | 20.431 | 31.336 | 28.505 | 1.00 | 14.95 | C |
| ATOM | 1700 | C | THR | B | 111 | 19.077 | 31.537 | 27.823 | 1.00 | 14.86 | C |
| ATOM | 1701 | O | THR | B | 111 | 18.720 | 32.705 | 27.696 | 1.00 | 18.62 | O |
| ATOM | 1702 | CB | THR | B | 111 | 20.254 | 30.986 | 30.016 | 1.00 | 10.83 | C |
| ATOM | 1703 | OG1 | THR | B | 111 | 19.440 | 32.008 | 30.536 | 1.00 | 14.58 | C |
| ATOM | 1704 | CG2 | THR | B | 111 | 21.520 | 31.006 | 30.845 | 1.00 | 11.33 | O |
| ATOM | 1705 | N | PRO | B | 112 | 18.205 | 30.602 | 27.418 | 1.00 | 14.14 | N |
| ATOM | 1706 | CA | PRO | B | 112 | 16.903 | 30.899 | 26.832 | 1.00 | 12.85 | C |
| ATOM | 1707 | C | PRO | B | 112 | 16.055 | 31.789 | 27.714 | 1.00 | 15.00 | C |
| ATOM | 1708 | O | PRO | B | 112 | 15.351 | 32.679 | 27.268 | 1.00 | 16.67 | O |
| ATOM | 1709 | CB | PRO | B | 112 | 16.297 | 29.536 | 26.730 | 1.00 | 13.18 | O |
| ATOM | 1710 | CG | PRO | B | 112 | 17.459 | 28.689 | 26.406 | 1.00 | 11.71 | O |
| ATOM | 1711 | CD | PRO | B | 112 | 18.482 | 29.179 | 27.402 | 1.00 | 12.63 | O |
| ATOM | 1712 | N | GLU | B | 113 | 16.103 | 31.597 | 29.015 | 1.00 | 17.42 | N |
| ATOM | 1713 | CA | GLU | B | 113 | 15.375 | 32.431 | 29.945 | 1.00 | 19.68 | C |
| ATOM | 1714 | C | GLU | B | 113 | 15.802 | 33.888 | 29.901 | 1.00 | 18.59 | C |
| ATOM | 1715 | O | GLU | B | 113 | 14.931 | 34.751 | 29.885 | 1.00 | 21.48 | O |
| ATOM | 1716 | CB | GLU | B | 113 | 15.546 | 31.841 | 31.328 | 1.00 | 22.92 | O |
| ATOM | 1717 | CG | GLU | B | 113 | 14.984 | 32.707 | 32.439 | 1.00 | 32.95 | O |
| ATOM | 1718 | CD | GLU | B | 113 | 15.763 | 32.704 | 33.770 | 1.00 | 39.93 | O |
| ATOM | 1719 | OE1 | GLU | B | 113 | 16.869 | 33.281 | 33.900 | 1.00 | 41.39 | O |
| ATOM | 1720 | OE2 | GLU | B | 113 | 15.193 | 32.144 | 34.712 | 1.00 | 44.90 | O |
| ATOM | 1721 | N | GLU | B | 114 | 17.096 | 34.210 | 29.885 | 1.00 | 18.49 | N |
| ATOM | 1722 | CA | GLU | B | 114 | 17.601 | 35.576 | 29.760 | 1.00 | 17.43 | C |
| ATOM | 1723 | C | GLU | B | 114 | 17.321 | 36.289 | 28.451 | 1.00 | 16.60 | C |
| ATOM | 1724 | O | GLU | B | 114 | 16.910 | 37.449 | 28.404 | 1.00 | 19.48 | O |
| ATOM | 1725 | CB | GLU | B | 114 | 19.090 | 35.543 | 29.980 | 1.00 | 19.55 | O |
| ATOM | 1726 | CG | GLU | B | 114 | 19.486 | 35.319 | 31.442 | 1.00 | 23.40 | O |
| ATOM | 1727 | CD | GLU | B | 114 | 20.962 | 35.034 | 31.718 | 1.00 | 25.98 | O |
| ATOM | 1728 | OE1 | GLU | B | 114 | 21.730 | 34.826 | 30.765 | 1.00 | 25.41 | O |
| ATOM | 1729 | OE2 | GLU | B | 114 | 21.322 | 34.982 | 32.906 | 1.00 | 28.77 | O |
| ATOM | 1730 | N | PHE | B | 115 | 17.507 | 35.551 | 27.379 | 1.00 | 14.86 | N |
| ATOM | 1731 | CA | PHE | B | 115 | 17.212 | 35.998 | 26.023 | 1.00 | 15.76 | C |
| ATOM | 1732 | C | PHE | B | 115 | 15.776 | 36.422 | 25.843 | 1.00 | 14.74 | C |
| ATOM | 1733 | O | PHE | B | 115 | 15.474 | 37.469 | 25.295 | 1.00 | 16.04 | O |
| ATOM | 1734 | CB | PHE | B | 115 | 17.513 | 34.865 | 25.012 | 1.00 | 14.37 | O |
| ATOM | 1735 | CG | PHE | B | 115 | 17.384 | 35.323 | 23.572 | 1.00 | 16.76 | C |
| ATOM | 1736 | CD1 | PHE | B | 115 | 18.400 | 36.062 | 22.990 | 1.00 | 15.08 | C |
| ATOM | 1737 | CD2 | PHE | B | 115 | 16.217 | 35.063 | 22.881 | 1.00 | 16.51 | C |
| ATOM | 1738 | CE1 | PHE | B | 115 | 18.169 | 36.611 | 21.755 | 1.00 | 15.92 | C |
| ATOM | 1739 | CE2 | PHE | B | 115 | 16.024 | 35.579 | 21.619 | 1.00 | 13.36 | C |
| ATOM | 1740 | CZ | PHE | B | 115 | 16.994 | 36.364 | 21.079 | 1.00 | 14.28 | C |
| ATOM | 1741 | N | PHE | B | 116 | 14.897 | 35.549 | 26.284 | 1.00 | 15.61 | N |
| ATOM | 1742 | CA | PHE | B | 116 | 13.497 | 35.810 | 26.150 | 1.00 | 15.94 | C |
| ATOM | 1743 | C | PHE | B | 116 | 12.918 | 36.798 | 27.125 | 1.00 | 16.92 | C |
| ATOM | 1744 | O | PHE | B | 116 | 11.842 | 37.326 | 26.862 | 1.00 | 18.97 | O |
| ATOM | 1745 | CB | PHE | B | 116 | 12.759 | 34.499 | 26.111 | 1.00 | 16.90 | C |

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FIGURE 8A-40

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1746 | CG | PHE | B | 116 | 12.962 | 33.796 | 24.776 | 1.00 | 16.87 | C |
| ATOM | 1747 | CD1 | PHE | B | 116 | 12.315 | 34.278 | 23.639 | 1.00 | 16.00 | C |
| ATOM | 1748 | CD2 | PHE | B | 116 | 13.830 | 32.714 | 24.689 | 1.00 | 17.13 | C |
| ATOM | 1749 | CE1 | PHE | B | 116 | 12.558 | 33.654 | 22.429 | 1.00 | 17.64 | C |
| ATOM | 1750 | CE2 | PHE | B | 116 | 14.079 | 32.114 | 23.482 | 1.00 | 16.31 | C |
| ATOM | 1751 | CZ | PHE | B | 116 | 13.427 | 32.582 | 22.349 | 1.00 | 17.77 | C |
| ATOM | 1752 | N | ARG | B | 117 | 13.629 | 37.094 | 28.208 | 1.00 | 17.01 | C |
| ATOM | 1753 | CA | ARG | B | 117 | 13.292 | 38.189 | 29.085 | 1.00 | 18.94 | N |
| ATOM | 1754 | C | ARG | B | 117 | 13.636 | 39.492 | 28.388 | 1.00 | 20.76 | C |
| ATOM | 1755 | O | ARG | B | 117 | 12.988 | 40.526 | 28.561 | 1.00 | 21.80 | C |
| ATOM | 1756 | CB | ARG | B | 117 | 14.124 | 38.043 | 30.361 | 1.00 | 22.28 | O |
| ATOM | 1757 | CG | ARG | B | 117 | 13.889 | 39.003 | 31.538 | 1.00 | 29.21 | C |
| ATOM | 1758 | CD | ARG | B | 117 | 13.292 | 38.359 | 32.834 | 1.00 | 35.23 | C |
| ATOM | 1759 | NE | ARG | B | 117 | 14.094 | 37.253 | 33.357 | 1.00 | 37.19 | N |
| ATOM | 1760 | CZ | ARG | B | 117 | 15.408 | 37.373 | 33.616 | 1.00 | 42.10 | N |
| ATOM | 1761 | NH1 | ARG | B | 117 | 16.023 | 38.568 | 33.647 | 1.00 | 45.58 | C |
| ATOM | 1762 | NH2 | ARG | B | 117 | 16.151 | 36.268 | 33.794 | 1.00 | 43.18 | N |
| ATOM | 1763 | N | ILE | B | 118 | 14.709 | 39.453 | 27.596 | 1.00 | 20.97 | N |
| ATOM | 1764 | CA | ILE | B | 118 | 15.078 | 40.588 | 26.807 | 1.00 | 18.77 | C |
| ATOM | 1765 | C | ILE | B | 118 | 14.103 | 40.799 | 25.662 | 1.00 | 20.54 | C |
| ATOM | 1766 | O | ILE | B | 118 | 13.592 | 41.896 | 25.487 | 1.00 | 20.49 | O |
| ATOM | 1767 | CB | ILE | B | 118 | 16.498 | 40.364 | 26.385 | 1.00 | 16.96 | C |
| ATOM | 1768 | CG1 | ILE | B | 118 | 17.377 | 40.504 | 27.587 | 1.00 | 12.82 | C |
| ATOM | 1769 | CG2 | ILE | B | 118 | 16.892 | 41.347 | 25.310 | 1.00 | 15.77 | C |
| ATOM | 1770 | CD1 | ILE | B | 118 | 18.851 | 40.271 | 27.253 | 1.00 | 14.00 | C |
| ATOM | 1771 | N | PHE | B | 119 | 13.817 | 39.736 | 24.922 | 1.00 | 22.16 | N |
| ATOM | 1772 | CA | PHE | B | 119 | 12.840 | 39.717 | 23.864 | 1.00 | 23.96 | C |
| ATOM | 1773 | C | PHE | B | 119 | 11.528 | 40.271 | 24.356 | 1.00 | 26.51 | C |
| ATOM | 1774 | O | PHE | B | 119 | 10.934 | 41.093 | 23.674 | 1.00 | 29.24 | C |
| ATOM | 1775 | CB | PHE | B | 119 | 12.660 | 38.299 | 23.364 | 1.00 | 22.84 | O |
| ATOM | 1776 | CG | PHE | B | 119 | 11.555 | 38.173 | 22.327 | 1.00 | 24.88 | C |
| ATOM | 1777 | CD1 | PHE | B | 119 | 11.811 | 38.512 | 21.006 | 1.00 | 25.69 | C |
| ATOM | 1778 | CD2 | PHE | B | 119 | 10.271 | 37.803 | 22.727 | 1.00 | 24.94 | C |
| ATOM | 1779 | CE1 | PHE | B | 119 | 10.748 | 38.539 | 20.122 | 1.00 | 25.07 | C |
| ATOM | 1780 | CE2 | PHE | B | 119 | 9.216 | 37.831 | 21.844 | 1.00 | 24.69 | C |
| ATOM | 1781 | CZ | PHE | B | 119 | 9.465 | 38.212 | 20.539 | 1.00 | 25.22 | C |
| ATOM | 1782 | N | ASN | B | 120 | 11.076 | 39.898 | 25.540 | 1.00 | 29.22 | N |
| ATOM | 1783 | CA | ASN | B | 120 | 9.863 | 40.470 | 26.094 | 1.00 | 31.04 | C |
| ATOM | 1784 | C | ASN | B | 120 | 9.953 | 41.939 | 26.499 | 1.00 | 32.79 | C |
| ATOM | 1785 | O | ASN | B | 120 | 9.018 | 42.684 | 26.204 | 1.00 | 34.41 | O |
| ATOM | 1786 | CB | ASN | B | 120 | 9.343 | 39.640 | 27.253 | 1.00 | 29.44 | C |
| ATOM | 1787 | CG | ASN | B | 120 | 8.856 | 38.301 | 26.738 | 1.00 | 33.04 | C |
| ATOM | 1788 | OD1 | ASN | B | 120 | 8.264 | 38.216 | 25.651 | 1.00 | 32.93 | O |
| ATOM | 1789 | ND2 | ASN | B | 120 | 9.110 | 37.237 | 27.508 | 1.00 | 31.91 | O |
| ATOM | 1790 | N | ARG | B | 121 | 11.018 | 42.436 | 27.140 | 1.00 | 32.47 | N |
| ATOM | 1791 | CA | ARG | B | 121 | 11.117 | 43.849 | 27.465 | 1.00 | 30.92 | C |
| ATOM | 1792 | C | ARG | B | 121 | 11.067 | 44.709 | 26.204 | 1.00 | 29.78 | C |
| ATOM | 1793 | O | ARG | B | 121 | 10.444 | 45.760 | 26.207 | 1.00 | 28.95 | C |
| ATOM | 1794 | CB | ARG | B | 121 | 12.391 | 44.075 | 28.271 | 1.00 | 33.61 | O |
| ATOM | 1795 | CG | ARG | B | 121 | 12.655 | 45.523 | 28.664 | 1.00 | 41.90 | C |
| ATOM | 1796 | CD | ARG | B | 121 | 11.463 | 46.261 | 29.336 | 1.00 | 48.78 | C |
| ATOM | 1797 | NE | ARG | B | 121 | 11.048 | 47.453 | 28.567 | 1.00 | 55.93 | N |
| ATOM | 1798 | CZ | ARG | B | 121 | 11.568 | 48.694 | 28.762 | 1.00 | 59.13 | N |
| ATOM | 1799 | NH1 | ARG | B | 121 | 12.543 | 48.894 | 29.659 | 1.00 | 60.86 | C |
| ATOM | 1800 | NH2 | ARG | B | 121 | 11.124 | 49.767 | 28.074 | 1.00 | 60.62 | N |
| ATOM | 1801 | N | SER | B | 122 | 11.680 | 44.225 | 25.121 | 1.00 | 29.04 | N |
| ATOM | 1802 | CA | SER | B | 122 | 11.818 | 44.920 | 23.854 | 1.00 | 27.66 | C |
| ATOM | 1803 | C | SER | B | 122 | 10.512 | 45.006 | 23.126 | 1.00 | 29.01 | C |
| ATOM | 1804 | O | SER | B | 122 | 10.198 | 46.085 | 22.634 | 1.00 | 30.77 | C |
| ATOM | 1805 | CB | SER | B | 122 | 12.808 | 44.195 | 22.954 | 1.00 | 24.91 | O |

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FIGURE 8A-41

| | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1806 | OG | SER | B | 122 | 14.125 | 44.237 | 23.464 | 1.00 | 21.03 |
| ATOM | 1807 | N | ILE | B | 123 | 9.765 | 43.896 | 23.061 | 1.00 | 30.73 |
| ATOM | 1808 | CA | ILE | B | 123 | 8.427 | 43.886 | 22.488 | 1.00 | 33.96 |
| ATOM | 1809 | C | ILE | B | 123 | 7.513 | 44.857 | 23.232 | 1.00 | 38.09 |
| ATOM | 1810 | O | ILE | B | 123 | 6.743 | 45.579 | 22.610 | 1.00 | 38.61 |
| ATOM | 1811 | CB | ILE | B | 123 | 7.863 | 42.445 | 22.513 | 1.00 | 33.36 |
| ATOM | 1812 | CG1 | ILE | B | 123 | 8.567 | 41.492 | 21.559 | 1.00 | 33.77 |
| ATOM | 1813 | CG2 | ILE | B | 123 | 6.385 | 42.334 | 22.276 | 1.00 | 35.01 |
| ATOM | 1814 | CD1 | ILE | B | 123 | 8.539 | 41.729 | 20.058 | 1.00 | 31.14 |
| ATOM | 1815 | N | ASP | B | 124 | 7.638 | 44.925 | 24.562 | 1.00 | 42.48 |
| ATOM | 1816 | CA | ASP | B | 124 | 6.868 | 45.809 | 25.424 | 1.00 | 45.69 |
| ATOM | 1817 | C | ASP | B | 124 | 7.347 | 47.237 | 25.404 | 1.00 | 45.68 |
| ATOM | 1818 | O | ASP | B | 124 | 6.592 | 48.118 | 25.836 | 1.00 | 46.88 |
| ATOM | 1819 | CB | ASP | B | 124 | 6.915 | 45.381 | 26.912 | 1.00 | 50.45 |
| ATOM | 1820 | CG | ASP | B | 124 | 6.483 | 43.950 | 27.274 | 1.00 | 56.00 |
| ATOM | 1821 | OD1 | ASP | B | 124 | 5.766 | 43.310 | 26.481 | 1.00 | 61.21 |
| ATOM | 1822 | OD2 | ASP | B | 124 | 6.883 | 43.461 | 28.344 | 1.00 | 56.72 |
| ATOM | 1823 | N | ALA | B | 125 | 8.599 | 47.461 | 24.970 | 1.00 | 46.60 |
| ATOM | 1824 | CA | ALA | B | 125 | 9.190 | 48.801 | 24.903 | 1.00 | 47.64 |
| ATOM | 1825 | C | ALA | B | 125 | 8.420 | 49.664 | 23.926 | 1.00 | 48.60 |
| ATOM | 1826 | O | ALA | B | 125 | 8.412 | 50.882 | 24.081 | 1.00 | 48.65 |
| ATOM | 1827 | CB | ALA | B | 125 | 10.643 | 48.781 | 24.422 | 1.00 | 46.01 |
| ATOM | 1828 | N | PHE | B | 126 | 7.752 | 49.014 | 22.960 | 1.00 | 50.56 |
| ATOM | 1829 | CA | PHE | B | 126 | 6.834 | 49.695 | 22.055 | 1.00 | 54.13 |
| ATOM | 1830 | C | PHE | B | 126 | 5.525 | 50.182 | 22.688 | 1.00 | 57.79 |
| ATOM | 1831 | O | PHE | B | 126 | 5.141 | 51.334 | 22.460 | 1.00 | 59.99 |
| ATOM | 1832 | CB | PHE | B | 126 | 6.538 | 48.850 | 20.810 | 1.00 | 51.52 |
| ATOM | 1833 | CG | PHE | B | 126 | 7.721 | 48.691 | 19.873 | 1.00 | 49.43 |
| ATOM | 1834 | CD1 | PHE | B | 126 | 8.650 | 47.685 | 20.086 | 1.00 | 48.93 |
| ATOM | 1835 | CD2 | PHE | B | 126 | 7.872 | 49.550 | 18.804 | 1.00 | 48.24 |
| ATOM | 1836 | CE1 | PHE | B | 126 | 9.721 | 47.531 | 19.226 | 1.00 | 47.28 |
| ATOM | 1837 | CE2 | PHE | B | 126 | 8.960 | 49.402 | 17.969 | 1.00 | 46.11 |
| ATOM | 1838 | CZ | PHE | B | 126 | 9.882 | 48.401 | 18.174 | 1.00 | 45.91 |
| ATOM | 1839 | N | LYS | B | 127 | 4.843 | 49.346 | 23.505 | 1.00 | 61.28 |
| ATOM | 1840 | CA | LYS | B | 127 | 3.558 | 49.636 | 24.178 | 1.00 | 62.20 |
| ATOM | 1841 | C | LYS | B | 127 | 3.454 | 50.906 | 25.026 | 1.00 | 62.03 |
| ATOM | 1842 | O | LYS | B | 127 | 2.394 | 51.539 | 25.092 | 1.00 | 61.71 |
| ATOM | 1843 | CB | LYS | B | 127 | 3.115 | 48.458 | 25.090 | 1.00 | 64.81 |
| ATOM | 1844 | CG | LYS | B | 127 | 2.463 | 47.185 | 24.502 | 1.00 | 65.92 |
| ATOM | 1845 | CD | LYS | B | 127 | 2.082 | 46.311 | 25.702 | 1.00 | 67.81 |
| ATOM | 1846 | CE | LYS | B | 127 | 2.369 | 44.834 | 25.433 | 1.00 | 69.44 |
| ATOM | 1847 | NZ | LYS | B | 127 | 2.594 | 44.129 | 26.691 | 1.00 | 68.14 |
| ATOM | 1848 | N | ASP | B | 128 | 4.561 | 51.200 | 25.719 | 1.00 | 62.76 |
| ATOM | 1849 | CA | ASP | B | 128 | 4.736 | 52.380 | 26.554 | 1.00 | 62.70 |
| ATOM | 1850 | C | ASP | B | 128 | 5.573 | 53.412 | 25.794 | 1.00 | 63.56 |
| ATOM | 1851 | O | ASP | B | 128 | 6.638 | 53.838 | 26.251 | 1.00 | 64.23 |
| ATOM | 1852 | CB | ASP | B | 128 | 5.480 | 51.925 | 27.833 | 1.00 | 62.32 |
| ATOM | 1853 | N | PHE | B | 129 | 5.128 | 53.802 | 24.587 | 1.00 | 64.47 |
| ATOM | 1854 | CA | PHE | B | 129 | 5.813 | 54.828 | 23.801 | 1.00 | 65.58 |
| ATOM | 1855 | C | PHE | B | 129 | 5.172 | 56.224 | 23.900 | 1.00 | 66.25 |
| ATOM | 1856 | O | PHE | B | 129 | 4.145 | 56.473 | 23.258 | 1.00 | 67.17 |
| ATOM | 1857 | CB | PHE | B | 129 | 5.971 | 54.368 | 22.338 | 1.00 | 64.56 |
| ATOM | 1858 | CG | PHE | B | 129 | 7.424 | 54.230 | 21.907 | 1.00 | 63.61 |
| ATOM | 1859 | CD1 | PHE | B | 129 | 8.187 | 55.356 | 21.634 | 1.00 | 64.45 |
| ATOM | 1860 | CD2 | PHE | B | 129 | 7.979 | 52.977 | 21.775 | 1.00 | 62.93 |
| ATOM | 1861 | CE1 | PHE | B | 129 | 9.503 | 55.219 | 21.235 | 1.00 | 64.07 |
| ATOM | 1862 | CE2 | PHE | B | 129 | 9.291 | 52.837 | 21.378 | 1.00 | 63.56 |
| ATOM | 1863 | CZ | PHE | B | 129 | 10.048 | 53.959 | 21.111 | 1.00 | 64.70 |
| ATOM | 1864 | N | ASP | B | 137 | 17.272 | 62.584 | 24.623 | 1.00 | 55.18 |
| ATOM | 1865 | CA | ASP | B | 137 | 18.560 | 63.025 | 24.106 | 1.00 | 54.96 |

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FIGURE 8A-42

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1866 | C | ASP | B | 137 | 19.597 | 61.931 | 23.769 | 1.00 | 55.95 | C |
| ATOM | 1867 | O | ASP | B | 137 | 20.291 | 62.026 | 22.743 | 1.00 | 55.11 | C |
| ATOM | 1868 | CB | ASP | B | 137 | 19.180 | 63.952 | 25.136 | 1.00 | 53.99 | C |
| ATOM | 1869 | N | CYS | B | 138 | 19.669 | 60.900 | 24.656 | 1.00 | 55.99 | N |
| ATOM | 1870 | CA | CYS | B | 138 | 20.594 | 59.741 | 24.665 | 1.00 | 55.50 | C |
| ATOM | 1871 | C | CYS | B | 138 | 22.065 | 59.964 | 25.031 | 1.00 | 55.10 | C |
| ATOM | 1872 | O | CYS | B | 138 | 22.723 | 58.973 | 25.357 | 1.00 | 55.77 | O |
| ATOM | 1873 | CB | CYS | B | 138 | 20.486 | 58.822 | 23.416 | 1.00 | 53.55 | O |
| ATOM | 1874 | SG | CYS | B | 138 | 18.766 | 58.362 | 23.058 | 1.00 | 53.01 | S |
| TER | 1876 | | CYS | B | 138 | | | | | | |
| ATOM | 1877 | N | ASN | C | 11 | 51.574 | 13.978 | 45.345 | 1.00 | 51.40 | N |
| ATOM | 1878 | CA | ASN | C | 11 | 50.150 | 14.075 | 45.169 | 1.00 | 50.61 | C |
| ATOM | 1879 | C | ASN | C | 11 | 49.636 | 15.080 | 46.231 | 1.00 | 51.75 | C |
| ATOM | 1880 | O | ASN | C | 11 | 49.446 | 16.244 | 45.828 | 1.00 | 52.28 | O |
| ATOM | 1881 | CB | ASN | C | 11 | 49.486 | 12.671 | 45.271 | 1.00 | 48.14 | C |
| ATOM | 1882 | N | VAL | C | 12 | 49.577 | 14.664 | 47.548 | 1.00 | 49.74 | N |
| ATOM | 1883 | CA | VAL | C | 12 | 48.941 | 15.269 | 48.771 | 1.00 | 46.17 | C |
| ATOM | 1884 | C | VAL | C | 12 | 49.317 | 16.681 | 49.255 | 1.00 | 43.47 | C |
| ATOM | 1885 | O | VAL | C | 12 | 48.526 | 17.397 | 49.868 | 1.00 | 42.02 | O |
| ATOM | 1886 | CB | VAL | C | 12 | 49.032 | 14.271 | 50.044 | 1.00 | 47.02 | C |
| ATOM | 1887 | CG1 | VAL | C | 12 | 50.479 | 14.042 | 50.561 | 1.00 | 46.01 | C |
| ATOM | 1888 | CG2 | VAL | C | 12 | 48.129 | 14.662 | 51.233 | 1.00 | 44.78 | C |
| ATOM | 1889 | N | LYS | C | 13 | 50.588 | 17.052 | 49.054 | 1.00 | 43.09 | N |
| ATOM | 1890 | CA | LYS | C | 13 | 51.082 | 18.424 | 49.218 | 1.00 | 39.49 | C |
| ATOM | 1891 | C | LYS | C | 13 | 50.370 | 19.321 | 48.180 | 1.00 | 36.49 | C |
| ATOM | 1892 | O | LYS | C | 13 | 49.910 | 20.435 | 48.472 | 1.00 | 35.14 | O |
| ATOM | 1893 | CB | LYS | C | 13 | 52.643 | 18.424 | 48.986 | 1.00 | 37.77 | C |
| ATOM | 1894 | N | ASP | C | 14 | 50.231 | 18.776 | 46.951 | 1.00 | 33.25 | N |
| ATOM | 1895 | CA | ASP | C | 14 | 49.522 | 19.456 | 45.898 | 1.00 | 27.29 | C |
| ATOM | 1896 | C | ASP | C | 14 | 48.042 | 19.262 | 45.991 | 1.00 | 21.51 | C |
| ATOM | 1897 | O | ASP | C | 14 | 47.408 | 20.205 | 45.602 | 1.00 | 20.53 | O |
| ATOM | 1898 | CB | ASP | C | 14 | 50.101 | 19.142 | 44.565 | 1.00 | 31.10 | C |
| ATOM | 1899 | CG | ASP | C | 14 | 51.439 | 19.856 | 44.288 | 1.00 | 35.88 | C |
| ATOM | 1900 | OD1 | ASP | C | 14 | 52.043 | 20.514 | 45.155 | 1.00 | 37.80 | C |
| ATOM | 1901 | OD2 | ASP | C | 14 | 51.890 | 19.755 | 43.143 | 1.00 | 37.19 | O |
| ATOM | 1902 | N | VAL | C | 15 | 47.447 | 18.202 | 46.526 | 1.00 | 15.89 | N |
| ATOM | 1903 | CA | VAL | C | 15 | 46.073 | 18.270 | 46.962 | 1.00 | 16.75 | C |
| ATOM | 1904 | C | VAL | C | 15 | 45.796 | 19.433 | 47.938 | 1.00 | 17.73 | C |
| ATOM | 1905 | O | VAL | C | 15 | 44.821 | 20.167 | 47.775 | 1.00 | 18.15 | O |
| ATOM | 1906 | CB | VAL | C | 15 | 45.653 | 16.905 | 47.548 | 1.00 | 17.03 | C |
| ATOM | 1907 | CG1 | VAL | C | 15 | 44.266 | 16.920 | 48.161 | 1.00 | 15.16 | C |
| ATOM | 1908 | CG2 | VAL | C | 15 | 45.656 | 15.889 | 46.430 | 1.00 | 17.49 | C |
| ATOM | 1909 | N | THR | C | 16 | 46.659 | 19.692 | 48.910 | 1.00 | 17.16 | N |
| ATOM | 1910 | CA | THR | C | 16 | 46.513 | 20.824 | 49.806 | 1.00 | 16.51 | C |
| ATOM | 1911 | C | THR | C | 16 | 46.660 | 22.151 | 49.096 | 1.00 | 15.07 | C |
| ATOM | 1912 | O | THR | C | 16 | 45.901 | 23.049 | 49.418 | 1.00 | 16.99 | O |
| ATOM | 1913 | CB | THR | C | 16 | 47.533 | 20.674 | 51.000 | 1.00 | 17.35 | C |
| ATOM | 1914 | OG1 | THR | C | 16 | 47.059 | 19.546 | 51.734 | 1.00 | 19.10 | O |
| ATOM | 1915 | CG2 | THR | C | 16 | 47.615 | 21.868 | 51.934 | 1.00 | 11.74 | C |
| ATOM | 1916 | N | LYS | C | 17 | 47.562 | 22.381 | 48.160 | 1.00 | 13.81 | N |
| ATOM | 1917 | CA | LYS | C | 17 | 47.496 | 23.602 | 47.390 | 1.00 | 15.88 | C |
| ATOM | 1918 | C | LYS | C | 17 | 46.197 | 23.789 | 46.541 | 1.00 | 16.97 | C |
| ATOM | 1919 | O | LYS | C | 17 | 45.608 | 24.877 | 46.465 | 1.00 | 17.88 | O |
| ATOM | 1920 | CB | LYS | C | 17 | 48.702 | 23.598 | 46.505 | 1.00 | 18.13 | C |
| ATOM | 1921 | CG | LYS | C | 17 | 50.006 | 23.615 | 47.257 | 1.00 | 21.24 | C |
| ATOM | 1922 | CD | LYS | C | 17 | 51.103 | 23.441 | 46.198 | 1.00 | 24.88 | C |
| ATOM | 1923 | CE | LYS | C | 17 | 52.486 | 23.537 | 46.798 | 1.00 | 28.59 | C |
| ATOM | 1924 | NZ | LYS | C | 17 | 52.730 | 24.883 | 47.284 | 1.00 | 31.31 | N |
| ATOM | 1925 | N | LEU | C | 18 | 45.682 | 22.736 | 45.880 | 1.00 | 14.39 | N |
| ATOM | 1926 | CA | LEU | C | 18 | 44.454 | 22.764 | 45.149 | 1.00 | 11.22 | C |

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FIGURE 8A-45

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2047 | CZ | TYR | C | 32 | 29.862 | 8.758 | 51.230 | 1.00 | 45.88 | C |
| ATOM | 2048 | OH | TYR | C | 32 | 30.238 | 8.549 | 52.557 | 1.00 | 49.38 | C |
| ATOM | 2049 | N | VAL | C | 33 | 29.391 | 6.459 | 46.718 | 1.00 | 46.10 | C |
| ATOM | 2050 | CA | VAL | C | 33 | 28.866 | 5.097 | 46.885 | 1.00 | 48.63 | C |
| ATOM | 2051 | C | VAL | C | 33 | 28.323 | 4.935 | 48.307 | 1.00 | 50.48 | C |
| ATOM | 2052 | O | VAL | C | 33 | 29.088 | 5.086 | 49.265 | 1.00 | 49.75 | C |
| ATOM | 2053 | CB | VAL | C | 33 | 29.900 | 4.000 | 46.501 | 1.00 | 49.02 | C |
| ATOM | 2054 | CG1 | VAL | C | 33 | 29.390 | 2.594 | 46.823 | 1.00 | 50.53 | C |
| ATOM | 2055 | CG2 | VAL | C | 33 | 30.216 | 4.072 | 45.014 | 1.00 | 47.63 | C |
| ATOM | 2056 | N | PRO | C | 34 | 27.006 | 4.682 | 48.505 | 1.00 | 53.28 | C |
| ATOM | 2057 | CA | PRO | C | 34 | 26.385 | 4.695 | 49.834 | 1.00 | 55.66 | C |
| ATOM | 2058 | C | PRO | C | 34 | 27.121 | 3.734 | 50.767 | 1.00 | 58.89 | C |
| ATOM | 2059 | O | PRO | C | 34 | 27.426 | 2.568 | 50.448 | 1.00 | 59.22 | C |
| ATOM | 2060 | CB | PRO | C | 34 | 24.936 | 4.297 | 49.549 | 1.00 | 54.96 | C |
| ATOM | 2061 | CG | PRO | C | 34 | 24.701 | 4.825 | 48.139 | 1.00 | 51.80 | C |
| ATOM | 2062 | CD | PRO | C | 34 | 26.002 | 4.428 | 47.456 | 1.00 | 51.86 | C |
| ATOM | 2063 | N | GLY | C | 35 | 27.545 | 4.399 | 51.850 | 1.00 | 60.51 | C |
| ATOM | 2064 | CA | GLY | C | 35 | 28.272 | 3.744 | 52.925 | 1.00 | 62.88 | C |
| ATOM | 2065 | C | GLY | C | 35 | 29.632 | 3.266 | 52.457 | 1.00 | 63.14 | C |
| ATOM | 2066 | O | GLY | C | 35 | 29.852 | 2.077 | 52.214 | 1.00 | 64.01 | C |
| HETATM | 2067 | N | MSE | C | 36 | 30.521 | 4.240 | 52.301 | 1.00 | 62.92 | C |
| HETATM | 2068 | CA | MSE | C | 36 | 31.881 | 3.970 | 51.881 | 1.00 | 63.09 | C |
| HETATM | 2069 | C | MSE | C | 36 | 32.945 | 4.485 | 52.836 | 1.00 | 64.77 | C |
| HETATM | 2070 | O | MSE | C | 36 | 34.148 | 4.357 | 52.599 | 1.00 | 65.03 | C |
| HETATM | 2071 | CB | MSE | C | 36 | 32.115 | 4.582 | 50.531 | 1.00 | 62.61 | C |
| HETATM | 2072 | CG | MSE | C | 36 | 31.973 | 6.068 | 50.551 | 1.00 | 60.55 | C |
| HETATM | 2073 | SE | MSE | C | 36 | 33.277 | 6.879 | 49.401 | 1.00 | 61.18 | C |
| HETATM | 2074 | CE | MSE | C | 36 | 34.541 | 7.346 | 50.777 | 1.00 | 55.15 | C |
| ATOM | 2075 | N | ASP | C | 37 | 32.430 | 5.163 | 53.863 | 1.00 | 66.73 | C |
| ATOM | 2076 | CA | ASP | C | 37 | 33.149 | 5.583 | 55.061 | 1.00 | 67.41 | C |
| ATOM | 2077 | C | ASP | C | 37 | 33.215 | 4.481 | 56.132 | 1.00 | 66.85 | C |
| ATOM | 2078 | O | ASP | C | 37 | 34.130 | 4.393 | 56.957 | 1.00 | 67.21 | C |
| ATOM | 2079 | CB | ASP | C | 37 | 32.478 | 6.867 | 55.589 | 1.00 | 69.00 | C |
| ATOM | 2080 | CG | ASP | C | 37 | 30.982 | 6.808 | 55.935 | 1.00 | 70.25 | C |
| ATOM | 2081 | OD1 | ASP | C | 37 | 30.143 | 6.538 | 55.061 | 1.00 | 69.81 | C |
| ATOM | 2082 | OD2 | ASP | C | 37 | 30.657 | 7.058 | 57.097 | 1.00 | 71.69 | C |
| ATOM | 2083 | N | VAL | C | 38 | 32.224 | 3.593 | 56.068 | 1.00 | 65.94 | C |
| ATOM | 2084 | CA | VAL | C | 38 | 32.091 | 2.461 | 56.960 | 1.00 | 64.55 | C |
| ATOM | 2085 | C | VAL | C | 38 | 32.395 | 1.200 | 56.170 | 1.00 | 65.94 | C |
| ATOM | 2086 | O | VAL | C | 38 | 33.340 | 0.521 | 56.584 | 1.00 | 68.33 | C |
| ATOM | 2087 | CB | VAL | C | 38 | 30.694 | 2.475 | 57.631 | 1.00 | 63.05 | C |
| ATOM | 2088 | CG1 | VAL | C | 38 | 29.960 | 1.135 | 57.787 | 1.00 | 62.73 | C |
| ATOM | 2089 | CG2 | VAL | C | 38 | 30.915 | 3.097 | 58.990 | 1.00 | 61.39 | C |
| ATOM | 2090 | N | LEU | C | 39 | 31.700 | 0.861 | 55.059 | 1.00 | 64.32 | C |
| ATOM | 2091 | CA | LEU | C | 39 | 31.997 | -0.365 | 54.328 | 1.00 | 63.23 | C |
| ATOM | 2092 | C | LEU | C | 39 | 33.487 | -0.412 | 53.952 | 1.00 | 62.57 | C |
| ATOM | 2093 | O | LEU | C | 39 | 34.084 | 0.647 | 53.713 | 1.00 | 63.24 | C |
| ATOM | 2094 | CB | LEU | C | 39 | 31.130 | -0.449 | 53.078 | 1.00 | 62.74 | C |
| ATOM | 2095 | N | PRO | C | 40 | 34.161 | -1.578 | 54.006 | 1.00 | 61.57 | C |
| ATOM | 2096 | CA | PRO | C | 40 | 35.608 | -1.719 | 53.761 | 1.00 | 59.74 | C |
| ATOM | 2097 | C | PRO | C | 40 | 36.009 | -1.462 | 52.318 | 1.00 | 57.52 | C |
| ATOM | 2098 | O | PRO | C | 40 | 35.183 | -1.629 | 51.418 | 1.00 | 54.10 | C |
| ATOM | 2099 | CB | PRO | C | 40 | 35.861 | -3.170 | 54.123 | 1.00 | 60.55 | C |
| ATOM | 2100 | CG | PRO | C | 40 | 34.550 | -3.863 | 53.762 | 1.00 | 60.74 | C |
| ATOM | 2101 | CD | PRO | C | 40 | 33.546 | -2.868 | 54.329 | 1.00 | 61.16 | C |
| ATOM | 2102 | N | SER | C | 41 | 37.282 | -1.110 | 52.111 | 1.00 | 56.39 | C |
| ATOM | 2103 | CA | SER | C | 41 | 37.779 | -0.735 | 50.798 | 1.00 | 56.77 | C |
| ATOM | 2104 | C | SER | C | 41 | 37.271 | -1.553 | 49.602 | 1.00 | 56.41 | C |
| ATOM | 2105 | O | SER | C | 41 | 36.627 | -0.992 | 48.727 | 1.00 | 56.58 | C |
| ATOM | 2106 | CB | SER | C | 41 | 39.292 | -0.643 | 50.831 | 1.00 | 57.36 | C |

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FIGURE 8A-46

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|----|
| ATOM | 2107 | OG | SER | C | 41 | 39.964 | -1.877 | 50.695 | 1.00 | 60.59 | O |
| ATOM | 2108 | N | HIS | C | 42 | 37.404 | -2.882 | 49.580 | 1.00 | 56.11 | ON |
| ATOM | 2109 | CA | HIS | C | 42 | 36.947 | -3.739 | 48.482 | 1.00 | 56.80 | C |
| ATOM | 2110 | C | HIS | C | 42 | 35.473 | -3.664 | 48.079 | 1.00 | 56.34 | C |
| ATOM | 2111 | O | HIS | C | 42 | 35.062 | -4.139 | 47.007 | 1.00 | 55.64 | O |
| ATOM | 2112 | CB | HIS | C | 42 | 37.301 | -5.217 | 48.795 | 1.00 | 60.78 | C |
| ATOM | 2113 | CG | HIS | C | 42 | 36.205 | -6.095 | 49.445 | 1.00 | 63.24 | C |
| ATOM | 2114 | ND1 | HIS | C | 42 | 35.894 | -6.211 | 50.736 | 1.00 | 63.50 | N |
| ATOM | 2115 | CD2 | HIS | C | 42 | 35.244 | -6.788 | 48.711 | 1.00 | 63.78 | C |
| ATOM | 2116 | CE1 | HIS | C | 42 | 34.762 | -6.882 | 50.802 | 1.00 | 64.65 | C |
| ATOM | 2117 | NE2 | HIS | C | 42 | 34.371 | -7.201 | 49.584 | 1.00 | 64.49 | N |
| ATOM | 2118 | N | CYS | C | 43 | 34.669 | -3.175 | 49.027 | 1.00 | 56.27 | N |
| ATOM | 2119 | CA | CYS | C | 43 | 33.239 | -3.012 | 48.806 | 1.00 | 56.25 | C |
| ATOM | 2120 | C | CYS | C | 43 | 32.953 | -1.871 | 47.844 | 1.00 | 54.69 | C |
| ATOM | 2121 | O | CYS | C | 43 | 32.104 | -2.006 | 46.959 | 1.00 | 56.17 | O |
| ATOM | 2122 | CB | CYS | C | 43 | 32.488 | -2.787 | 50.120 | 1.00 | 57.47 | C |
| ATOM | 2123 | SG | CYS | C | 43 | 31.647 | -4.253 | 50.786 | 1.00 | 60.51 | S |
| ATOM | 2124 | N | TRP | C | 44 | 33.695 | -0.765 | 47.973 | 1.00 | 51.41 | N |
| ATOM | 2125 | CA | TRP | C | 44 | 33.338 | 0.464 | 47.287 | 1.00 | 47.58 | C |
| ATOM | 2126 | C | TRP | C | 44 | 34.349 | 0.946 | 46.300 | 1.00 | 46.08 | C |
| ATOM | 2127 | O | TRP | C | 44 | 33.969 | 1.593 | 45.341 | 1.00 | 46.29 | O |
| ATOM | 2128 | CB | TRP | C | 44 | 33.089 | 1.587 | 48.271 | 1.00 | 47.09 | C |
| ATOM | 2129 | CG | TRP | C | 44 | 34.199 | 1.801 | 49.301 | 1.00 | 46.63 | C |
| ATOM | 2130 | CD1 | TRP | C | 44 | 34.221 | 1.046 | 50.444 | 1.00 | 47.77 | CC |
| ATOM | 2131 | CD2 | TRP | C | 44 | 35.261 | 2.660 | 49.225 | 1.00 | 45.55 | C |
| ATOM | 2132 | NE1 | TRP | C | 44 | 35.307 | 1.419 | 51.078 | 1.00 | 47.46 | C |
| ATOM | 2133 | CE2 | TRP | C | 44 | 35.948 | 2.361 | 50.389 | 1.00 | 44.86 | CC |
| ATOM | 2134 | CE3 | TRP | C | 44 | 35.723 | 3.640 | 48.403 | 1.00 | 42.70 | CC |
| ATOM | 2135 | CZ2 | TRP | C | 44 | 37.122 | 2.956 | 50.754 | 1.00 | 43.79 | CC |
| ATOM | 2136 | CZ3 | TRP | C | 44 | 36.886 | 4.263 | 48.782 | 1.00 | 43.82 | CC |
| ATOM | 2137 | CH2 | TRP | C | 44 | 37.597 | 3.925 | 49.920 | 1.00 | 42.91 | CC |
| ATOM | 2138 | N | ILE | C | 45 | 35.615 | 0.635 | 46.539 | 1.00 | 45.14 | CC |
| ATOM | 2139 | CA | ILE | C | 45 | 36.735 | 1.252 | 45.851 | 1.00 | 47.08 | CC |
| ATOM | 2140 | C | ILE | C | 45 | 36.657 | 1.198 | 44.329 | 1.00 | 47.61 | CC |
| ATOM | 2141 | O | ILE | C | 45 | 36.955 | 2.157 | 43.619 | 1.00 | 48.87 | CC |
| ATOM | 2142 | CB | ILE | C | 45 | 38.085 | 0.681 | 46.427 | 1.00 | 47.91 | CC |
| ATOM | 2143 | CG1 | ILE | C | 45 | 39.316 | 1.515 | 46.123 | 1.00 | 46.35 | CC |
| ATOM | 2144 | CG2 | ILE | C | 45 | 38.420 | -0.723 | 45.905 | 1.00 | 50.05 | CC |
| ATOM | 2145 | CD1 | ILE | C | 45 | 39.180 | 2.995 | 46.462 | 1.00 | 43.72 | CC |
| ATOM | 2146 | N | SER | C | 46 | 36.158 | 0.077 | 43.850 | 1.00 | 47.61 | CC |
| ATOM | 2147 | CA | SER | C | 46 | 36.069 | -0.245 | 42.437 | 1.00 | 48.09 | CC |
| ATOM | 2148 | C | SER | C | 46 | 35.166 | 0.685 | 41.595 | 1.00 | 47.26 | CC |
| ATOM | 2149 | O | SER | C | 46 | 35.598 | 1.186 | 40.555 | 1.00 | 46.49 | CC |
| ATOM | 2150 | CB | SER | C | 46 | 35.688 | -1.728 | 42.427 | 1.00 | 50.90 | CC |
| ATOM | 2151 | OG | SER | C | 46 | 35.093 | -2.219 | 43.664 | 1.00 | 54.24 | CC |
| ATOM | 2152 | N | GLU | C | 47 | 33.932 | 0.997 | 42.039 | 1.00 | 46.80 | O |
| ATOM | 2153 | CA | GLU | C | 47 | 33.095 | 2.037 | 41.430 | 1.00 | 45.94 | O |
| ATOM | 2154 | C | GLU | C | 47 | 33.599 | 3.449 | 41.776 | 1.00 | 43.82 | O |
| ATOM | 2155 | O | GLU | C | 47 | 33.532 | 4.348 | 40.947 | 1.00 | 43.16 | O |
| ATOM | 2156 | CB | GLU | C | 47 | 31.602 | 1.843 | 41.831 | 1.00 | 47.29 | O |
| ATOM | 2157 | CG | GLU | C | 47 | 30.478 | 2.752 | 41.246 | 1.00 | 52.00 | O |
| ATOM | 2158 | CD | GLU | C | 47 | 29.748 | 2.394 | 39.936 | 1.00 | 54.16 | O |
| ATOM | 2159 | OE1 | GLU | C | 47 | 28.894 | 1.494 | 39.926 | 1.00 | 57.21 | O |
| ATOM | 2160 | OE2 | GLU | C | 47 | 29.989 | 3.052 | 38.922 | 1.00 | 54.36 | O |
| HETATM | 2161 | N | MSE | C | 48 | 34.170 | 3.670 | 42.967 | 1.00 | 43.01 | O |
| HETATM | 2162 | CA | MSE | C | 48 | 34.601 | 4.979 | 43.448 | 1.00 | 40.77 | N |
| HETATM | 2163 | C | MSE | C | 48 | 35.795 | 5.538 | 42.724 | 1.00 | 37.10 | C |
| HETATM | 2164 | O | MSE | C | 48 | 35.799 | 6.739 | 42.563 | 1.00 | 39.16 | O |
| HETATM | 2165 | CB | MSE | C | 48 | 34.926 | 4.968 | 44.927 | 1.00 | 43.83 | O |
| HETATM | 2166 | CG | MSE | C | 48 | 34.667 | 6.334 | 45.551 | 1.00 | 49.60 | C |

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FIGURE 8A-47

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|----|
| HETATM | 2167 | SE | MSE | C | 48 | 32.809 | 6.850 | 45.340 | 1.00 | 57.46 | SE |
| HETATM | 2168 | CE | MSE | C | 48 | 32.917 | 8.464 | 46.266 | 1.00 | 52.90 | C |
| ATOM | 2169 | N | VAL | C | 49 | 36.793 | 4.773 | 42.266 | 1.00 | 34.29 | N |
| ATOM | 2170 | CA | VAL | C | 49 | 37.855 | 5.271 | 41.388 | 1.00 | 30.22 | C |
| ATOM | 2171 | C | VAL | C | 49 | 37.372 | 5.680 | 39.997 | 1.00 | 31.03 | C |
| ATOM | 2172 | O | VAL | C | 49 | 37.936 | 6.572 | 39.365 | 1.00 | 30.17 | O |
| ATOM | 2173 | CB | VAL | C | 49 | 39.021 | 4.288 | 41.268 | 1.00 | 27.65 | C |
| ATOM | 2174 | CG1 | VAL | C | 49 | 39.719 | 4.131 | 42.581 | 1.00 | 27.80 | C |
| ATOM | 2175 | CG2 | VAL | C | 49 | 38.591 | 2.924 | 40.828 | 1.00 | 27.38 | C |
| ATOM | 2176 | N | VAL | C | 50 | 36.319 | 5.056 | 39.478 | 1.00 | 29.68 | N |
| ATOM | 2177 | CA | VAL | C | 50 | 35.727 | 5.548 | 38.255 | 1.00 | 29.53 | C |
| ATOM | 2178 | C | VAL | C | 50 | 34.932 | 6.806 | 38.559 | 1.00 | 28.57 | C |
| ATOM | 2179 | O | VAL | C | 50 | 35.069 | 7.755 | 37.800 | 1.00 | 30.41 | O |
| ATOM | 2180 | CB | VAL | C | 50 | 34.904 | 4.446 | 37.554 | 1.00 | 30.06 | C |
| ATOM | 2181 | CG1 | VAL | C | 50 | 34.026 | 4.900 | 36.371 | 1.00 | 28.50 | C |
| ATOM | 2182 | CG2 | VAL | C | 50 | 35.916 | 3.457 | 37.070 | 1.00 | 29.52 | C |
| ATOM | 2183 | N | GLN | C | 51 | 34.147 | 6.917 | 39.639 | 1.00 | 28.05 | N |
| ATOM | 2184 | CA | GLN | C | 51 | 33.421 | 8.148 | 39.945 | 1.00 | 27.55 | C |
| ATOM | 2185 | C | GLN | C | 51 | 34.267 | 9.336 | 40.379 | 1.00 | 26.77 | C |
| ATOM | 2186 | O | GLN | C | 51 | 33.957 | 10.480 | 40.061 | 1.00 | 27.78 | O |
| ATOM | 2187 | CB | GLN | C | 51 | 32.276 | 7.962 | 40.944 | 1.00 | 27.95 | C |
| ATOM | 2188 | CG | GLN | C | 51 | 31.142 | 7.029 | 40.503 | 1.00 | 31.66 | C |
| ATOM | 2189 | CD | GLN | C | 51 | 30.518 | 7.274 | 39.121 | 1.00 | 35.14 | C |
| ATOM | 2190 | OE1 | GLN | C | 51 | 30.531 | 8.353 | 38.510 | 1.00 | 34.94 | O |
| ATOM | 2191 | NE2 | GLN | C | 51 | 29.945 | 6.214 | 38.566 | 1.00 | 36.11 | O |
| ATOM | 2192 | N | LEU | C | 52 | 35.349 | 9.130 | 41.113 | 1.00 | 24.84 | N |
| ATOM | 2193 | CA | LEU | C | 52 | 36.290 | 10.188 | 41.316 | 1.00 | 24.73 | C |
| ATOM | 2194 | C | LEU | C | 52 | 36.914 | 10.560 | 40.004 | 1.00 | 25.82 | C |
| ATOM | 2195 | O | LEU | C | 52 | 37.061 | 11.752 | 39.750 | 1.00 | 26.91 | O |
| ATOM | 2196 | CB | LEU | C | 52 | 37.349 | 9.754 | 42.251 | 1.00 | 25.92 | C |
| ATOM | 2197 | CG | LEU | C | 52 | 36.831 | 9.701 | 43.653 | 1.00 | 27.26 | C |
| ATOM | 2198 | CD1 | LEU | C | 52 | 37.880 | 9.090 | 44.510 | 1.00 | 27.86 | C |
| ATOM | 2199 | CD2 | LEU | C | 52 | 36.473 | 11.078 | 44.141 | 1.00 | 27.93 | C |
| ATOM | 2200 | N | SER | C | 53 | 37.211 | 9.566 | 39.148 | 1.00 | 27.18 | N |
| ATOM | 2201 | CA | SER | C | 53 | 37.788 | 9.790 | 37.838 | 1.00 | 24.69 | C |
| ATOM | 2202 | C | SER | C | 53 | 36.859 | 10.558 | 36.918 | 1.00 | 26.00 | C |
| ATOM | 2203 | O | SER | C | 53 | 37.336 | 11.388 | 36.166 | 1.00 | 26.97 | O |
| ATOM | 2204 | CB | SER | C | 53 | 38.172 | 8.499 | 37.198 | 1.00 | 25.64 | C |
| ATOM | 2205 | OG | SER | C | 53 | 38.902 | 8.772 | 36.019 | 1.00 | 24.45 | O |
| ATOM | 2206 | N | ASP | C | 54 | 35.544 | 10.421 | 36.932 | 1.00 | 27.50 | N |
| ATOM | 2207 | CA | ASP | C | 54 | 34.743 | 11.292 | 36.113 | 1.00 | 29.13 | C |
| ATOM | 2208 | C | ASP | C | 54 | 34.719 | 12.679 | 36.663 | 1.00 | 27.20 | C |
| ATOM | 2209 | O | ASP | C | 54 | 34.826 | 13.616 | 35.906 | 1.00 | 30.75 | O |
| ATOM | 2210 | CB | ASP | C | 54 | 33.314 | 10.874 | 36.099 | 1.00 | 35.74 | C |
| ATOM | 2211 | CG | ASP | C | 54 | 33.056 | 9.521 | 35.502 | 1.00 | 43.27 | C |
| ATOM | 2212 | OD1 | ASP | C | 54 | 33.871 | 9.016 | 34.694 | 1.00 | 44.80 | O |
| ATOM | 2213 | OD2 | ASP | C | 54 | 31.996 | 8.988 | 35.876 | 1.00 | 47.24 | O |
| ATOM | 2214 | N | SER | C | 55 | 34.554 | 12.829 | 37.966 | 1.00 | 26.41 | N |
| ATOM | 2215 | CA | SER | C | 55 | 34.470 | 14.119 | 38.610 | 1.00 | 23.34 | C |
| ATOM | 2216 | C | SER | C | 55 | 35.676 | 14.964 | 38.382 | 1.00 | 19.99 | C |
| ATOM | 2217 | O | SER | C | 55 | 35.544 | 16.157 | 38.175 | 1.00 | 20.42 | O |
| ATOM | 2218 | CB | SER | C | 55 | 34.306 | 13.948 | 40.105 | 1.00 | 24.40 | C |
| ATOM | 2219 | OG | SER | C | 55 | 33.079 | 13.321 | 40.431 | 1.00 | 24.29 | O |
| ATOM | 2220 | N | LEU | C | 56 | 36.837 | 14.338 | 38.432 | 1.00 | 19.40 | N |
| ATOM | 2221 | CA | LEU | C | 56 | 38.082 | 15.062 | 38.245 | 1.00 | 21.98 | C |
| ATOM | 2222 | C | LEU | C | 56 | 38.333 | 15.488 | 36.797 | 1.00 | 23.22 | C |
| ATOM | 2223 | O | LEU | C | 56 | 38.922 | 16.543 | 36.512 | 1.00 | 21.76 | O |
| ATOM | 2224 | CB | LEU | C | 56 | 39.301 | 14.271 | 38.793 | 1.00 | 21.06 | C |
| ATOM | 2225 | CG | LEU | C | 56 | 39.614 | 14.342 | 40.291 | 1.00 | 19.56 | C |
| ATOM | 2226 | CD1 | LEU | C | 56 | 40.647 | 13.313 | 40.678 | 1.00 | 18.16 | C |

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FIGURE 8A-48

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2227 | CD2 | LEU | C | 56 | 40.132 | 15.717 | 40.651 | 1.00 | 16.61 | C |
| ATOM | 2228 | N | THR | C | 57 | 37.873 | 14.624 | 35.881 | 1.00 | 25.77 | N |
| ATOM | 2229 | CA | THR | C | 57 | 37.991 | 14.906 | 34.462 | 1.00 | 28.23 | C |
| ATOM | 2230 | C | THR | C | 57 | 37.020 | 16.004 | 34.104 | 1.00 | 28.03 | C |
| ATOM | 2231 | O | THR | C | 57 | 37.390 | 16.908 | 33.364 | 1.00 | 31.55 | C |
| ATOM | 2232 | CB | THR | C | 57 | 37.813 | 13.669 | 33.596 | 1.00 | 30.08 | O |
| ATOM | 2233 | OG1 | THR | C | 57 | 38.904 | 12.849 | 33.972 | 1.00 | 32.28 | C |
| ATOM | 2234 | CG2 | THR | C | 57 | 38.044 | 13.945 | 32.109 | 1.00 | 33.98 | O |
| ATOM | 2235 | N | ASP | C | 58 | 35.831 | 16.009 | 34.675 | 1.00 | 26.77 | N |
| ATOM | 2236 | CA | ASP | C | 58 | 34.940 | 17.120 | 34.486 | 1.00 | 29.31 | C |
| ATOM | 2237 | C | ASP | C | 58 | 35.387 | 18.422 | 35.173 | 1.00 | 28.49 | C |
| ATOM | 2238 | O | ASP | C | 58 | 35.241 | 19.515 | 34.614 | 1.00 | 29.44 | C |
| ATOM | 2239 | CB | ASP | C | 58 | 33.489 | 16.679 | 34.870 | 1.00 | 36.00 | O |
| ATOM | 2240 | CG | ASP | C | 58 | 32.849 | 15.532 | 34.032 | 1.00 | 40.53 | C |
| ATOM | 2241 | OD1 | ASP | C | 58 | 33.503 | 14.924 | 33.151 | 1.00 | 41.90 | O |
| ATOM | 2242 | OD2 | ASP | C | 58 | 31.673 | 15.229 | 34.294 | 1.00 | 42.29 | O |
| ATOM | 2243 | N | LEU | C | 59 | 35.964 | 18.350 | 36.383 | 1.00 | 26.07 | N |
| ATOM | 2244 | CA | LEU | C | 59 | 36.486 | 19.508 | 37.074 | 1.00 | 21.52 | C |
| ATOM | 2245 | C | LEU | C | 59 | 37.611 | 20.115 | 36.285 | 1.00 | 19.04 | C |
| ATOM | 2246 | O | LEU | C | 59 | 37.748 | 21.317 | 36.312 | 1.00 | 20.31 | C |
| ATOM | 2247 | CB | LEU | C | 59 | 37.028 | 19.118 | 38.444 | 1.00 | 19.27 | C |
| ATOM | 2248 | CG | LEU | C | 59 | 37.519 | 20.223 | 39.377 | 1.00 | 18.52 | C |
| ATOM | 2249 | CD1 | LEU | C | 59 | 36.411 | 21.181 | 39.805 | 1.00 | 14.85 | C |
| ATOM | 2250 | CD2 | LEU | C | 59 | 38.147 | 19.538 | 40.574 | 1.00 | 18.90 | C |
| ATOM | 2251 | N | LEU | C | 60 | 38.399 | 19.348 | 35.553 | 1.00 | 19.17 | C |
| ATOM | 2252 | CA | LEU | C | 60 | 39.549 | 19.854 | 34.840 | 1.00 | 20.10 | N |
| ATOM | 2253 | C | LEU | C | 60 | 39.173 | 20.833 | 33.766 | 1.00 | 22.23 | C |
| ATOM | 2254 | O | LEU | C | 60 | 39.912 | 21.768 | 33.474 | 1.00 | 24.00 | C |
| ATOM | 2255 | CB | LEU | C | 60 | 40.290 | 18.718 | 34.206 | 1.00 | 18.56 | C |
| ATOM | 2256 | CG | LEU | C | 60 | 41.582 | 19.115 | 33.520 | 1.00 | 19.76 | C |
| ATOM | 2257 | CD1 | LEU | C | 60 | 42.638 | 19.404 | 34.561 | 1.00 | 17.43 | C |
| ATOM | 2258 | CD2 | LEU | C | 60 | 42.018 | 18.002 | 32.555 | 1.00 | 20.53 | C |
| ATOM | 2259 | N | ASP | C | 61 | 37.984 | 20.629 | 33.214 | 1.00 | 25.53 | N |
| ATOM | 2260 | CA | ASP | C | 61 | 37.471 | 21.478 | 32.157 | 1.00 | 27.32 | C |
| ATOM | 2261 | C | ASP | C | 61 | 36.950 | 22.809 | 32.666 | 1.00 | 24.92 | C |
| ATOM | 2262 | O | ASP | C | 61 | 36.768 | 23.738 | 31.883 | 1.00 | 26.04 | C |
| ATOM | 2263 | CB | ASP | C | 61 | 36.365 | 20.729 | 31.389 | 1.00 | 35.92 | C |
| ATOM | 2264 | CG | ASP | C | 61 | 36.753 | 19.367 | 30.759 | 1.00 | 45.09 | C |
| ATOM | 2265 | OD1 | ASP | C | 61 | 37.808 | 19.241 | 30.086 | 1.00 | 48.21 | C |
| ATOM | 2266 | OD2 | ASP | C | 61 | 35.970 | 18.414 | 30.956 | 1.00 | 49.47 | O |
| ATOM | 2267 | N | LYS | C | 62 | 36.733 | 22.956 | 33.979 | 1.00 | 22.12 | N |
| ATOM | 2268 | CA | LYS | C | 62 | 36.379 | 24.234 | 34.559 | 1.00 | 18.62 | C |
| ATOM | 2269 | C | LYS | C | 62 | 37.603 | 25.082 | 34.727 | 1.00 | 17.52 | C |
| ATOM | 2270 | O | LYS | C | 62 | 37.491 | 26.205 | 35.176 | 1.00 | 19.68 | C |
| ATOM | 2271 | CB | LYS | C | 62 | 35.718 | 24.064 | 35.888 | 1.00 | 17.21 | C |
| ATOM | 2272 | CG | LYS | C | 62 | 34.590 | 23.048 | 35.893 | 1.00 | 20.59 | C |
| ATOM | 2273 | CD | LYS | C | 62 | 33.552 | 23.302 | 34.802 | 1.00 | 23.94 | C |
| ATOM | 2274 | CE | LYS | C | 62 | 32.302 | 22.398 | 34.907 | 1.00 | 27.69 | C |
| ATOM | 2275 | NZ | LYS | C | 62 | 32.621 | 20.990 | 35.112 | 1.00 | 33.53 | C |
| ATOM | 2276 | N | PHE | C | 63 | 38.792 | 24.629 | 34.385 | 1.00 | 16.95 | N |
| ATOM | 2277 | CA | PHE | C | 63 | 39.980 | 25.398 | 34.650 | 1.00 | 18.75 | N |
| ATOM | 2278 | C | PHE | C | 63 | 40.714 | 25.584 | 33.363 | 1.00 | 20.52 | C |
| ATOM | 2279 | O | PHE | C | 63 | 40.491 | 24.894 | 32.375 | 1.00 | 22.83 | C |
| ATOM | 2280 | CB | PHE | C | 63 | 40.890 | 24.728 | 35.712 | 1.00 | 16.49 | C |
| ATOM | 2281 | CG | PHE | C | 63 | 40.280 | 24.790 | 37.109 | 1.00 | 15.86 | C |
| ATOM | 2282 | CD1 | PHE | C | 63 | 40.413 | 25.931 | 37.893 | 1.00 | 15.21 | C |
| ATOM | 2283 | CD2 | PHE | C | 63 | 39.475 | 23.764 | 37.555 | 1.00 | 16.14 | C |
| ATOM | 2284 | CE1 | PHE | C | 63 | 39.717 | 26.070 | 39.078 | 1.00 | 11.64 | C |
| ATOM | 2285 | CE2 | PHE | C | 63 | 38.742 | 23.932 | 38.732 | 1.00 | 17.01 | C |
| ATOM | 2286 | CZ | PHE | C | 63 | 38.864 | 25.086 | 39.487 | 1.00 | 11.68 | C |

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FIGURE 8A-50

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2347 | CG | ASN | C | 72 | 43.443 | 25.398 | 40.958 | 1.00 | 16.98 |
| ATOM | 2348 | OD1 | ASN | C | 72 | 44.439 | 25.399 | 41.698 | 1.00 | 15.50 |
| ATOM | 2349 | ND2 | ASN | C | 72 | 42.348 | 26.051 | 41.315 | 1.00 | 16.58 |
| ATOM | 2350 | N | TYR | C | 73 | 44.626 | 23.493 | 36.878 | 1.00 | 17.45 |
| ATOM | 2351 | CA | TYR | C | 73 | 44.546 | 22.649 | 35.715 | 1.00 | 16.35 |
| ATOM | 2352 | C | TYR | C | 73 | 45.628 | 21.603 | 35.846 | 1.00 | 16.88 |
| ATOM | 2353 | O | TYR | C | 73 | 45.388 | 20.407 | 35.803 | 1.00 | 18.90 |
| ATOM | 2354 | CB | TYR | C | 73 | 44.797 | 23.540 | 34.503 | 1.00 | 14.79 |
| ATOM | 2355 | CG | TYR | C | 73 | 44.618 | 22.779 | 33.215 | 1.00 | 18.01 |
| ATOM | 2356 | CD1 | TYR | C | 73 | 45.649 | 22.000 | 32.745 | 1.00 | 18.75 |
| ATOM | 2357 | CD2 | TYR | C | 73 | 43.428 | 22.809 | 32.544 | 1.00 | 17.80 |
| ATOM | 2358 | CE1 | TYR | C | 73 | 45.507 | 21.189 | 31.632 | 1.00 | 23.12 |
| ATOM | 2359 | CE2 | TYR | C | 73 | 43.282 | 22.000 | 31.424 | 1.00 | 23.77 |
| ATOM | 2360 | CZ | TYR | C | 73 | 44.300 | 21.160 | 30.987 | 1.00 | 22.85 |
| ATOM | 2361 | OH | TYR | C | 73 | 44.105 | 20.242 | 29.959 | 1.00 | 27.47 |
| ATOM | 2362 | N | SER | C | 74 | 46.846 | 22.071 | 36.054 | 1.00 | 19.27 |
| ATOM | 2363 | CA | SER | C | 74 | 48.037 | 21.234 | 36.196 | 1.00 | 18.80 |
| ATOM | 2364 | C | SER | C | 74 | 47.939 | 20.205 | 37.316 | 1.00 | 18.49 |
| ATOM | 2365 | O | SER | C | 74 | 48.192 | 19.026 | 37.062 | 1.00 | 18.14 |
| ATOM | 2366 | CB | SER | C | 74 | 49.160 | 22.197 | 36.410 | 1.00 | 19.97 |
| ATOM | 2367 | OG | SER | C | 74 | 50.345 | 21.552 | 36.749 | 1.00 | 27.05 |
| ATOM | 2368 | N | ILE | C | 75 | 47.536 | 20.603 | 38.532 | 1.00 | 17.15 |
| ATOM | 2369 | CA | ILE | C | 75 | 47.360 | 19.670 | 39.640 | 1.00 | 15.78 |
| ATOM | 2370 | C | ILE | C | 75 | 46.266 | 18.688 | 39.303 | 1.00 | 15.56 |
| ATOM | 2371 | O | ILE | C | 75 | 46.392 | 17.487 | 39.540 | 1.00 | 15.90 |
| ATOM | 2372 | CB | ILE | C | 75 | 47.004 | 20.373 | 40.994 | 1.00 | 14.47 |
| ATOM | 2373 | CG1 | ILE | C | 75 | 48.069 | 21.396 | 41.311 | 1.00 | 15.08 |
| ATOM | 2374 | CG2 | ILE | C | 75 | 46.847 | 19.406 | 42.151 | 1.00 | 9.44 |
| ATOM | 2375 | CD1 | ILE | C | 75 | 47.662 | 22.494 | 42.334 | 1.00 | 16.06 |
| ATOM | 2376 | N | ILE | C | 76 | 45.174 | 19.165 | 38.739 | 1.00 | 15.87 |
| ATOM | 2377 | CA | ILE | C | 76 | 44.072 | 18.254 | 38.540 | 1.00 | 16.45 |
| ATOM | 2378 | C | ILE | C | 76 | 44.423 | 17.278 | 37.416 | 1.00 | 18.42 |
| ATOM | 2379 | O | ILE | C | 76 | 44.047 | 16.107 | 37.479 | 1.00 | 21.96 |
| ATOM | 2380 | CB | ILE | C | 76 | 42.777 | 19.029 | 38.276 | 1.00 | 16.99 |
| ATOM | 2381 | CG1 | ILE | C | 76 | 42.407 | 20.014 | 39.366 | 1.00 | 18.36 |
| ATOM | 2382 | CG2 | ILE | C | 76 | 41.661 | 18.026 | 38.294 | 1.00 | 18.72 |
| ATOM | 2383 | CD1 | ILE | C | 76 | 41.376 | 21.090 | 38.981 | 1.00 | 13.71 |
| ATOM | 2384 | N | ASP | C | 77 | 45.169 | 17.686 | 36.395 | 1.00 | 19.28 |
| ATOM | 2385 | CA | ASP | C | 77 | 45.673 | 16.806 | 35.340 | 1.00 | 20.35 |
| ATOM | 2386 | C | ASP | C | 77 | 46.477 | 15.616 | 35.867 | 1.00 | 18.75 |
| ATOM | 2387 | O | ASP | C | 77 | 46.259 | 14.474 | 35.483 | 1.00 | 20.55 |
| ATOM | 2388 | CB | ASP | C | 77 | 46.528 | 17.679 | 34.388 | 1.00 | 23.72 |
| ATOM | 2389 | CG | ASP | C | 77 | 46.796 | 17.143 | 32.984 | 1.00 | 27.17 |
| ATOM | 2390 | OD1 | ASP | C | 77 | 46.195 | 16.148 | 32.611 | 1.00 | 29.11 |
| ATOM | 2391 | OD2 | ASP | C | 77 | 47.586 | 17.723 | 32.239 | 1.00 | 31.91 |
| ATOM | 2392 | N | LYS | C | 78 | 47.401 | 15.826 | 36.791 | 1.00 | 18.00 |
| ATOM | 2393 | CA | LYS | C | 78 | 48.064 | 14.729 | 37.494 | 1.00 | 19.18 |
| ATOM | 2394 | C | LYS | C | 78 | 47.114 | 13.802 | 38.229 | 1.00 | 16.84 |
| ATOM | 2395 | O | LYS | C | 78 | 47.200 | 12.586 | 38.170 | 1.00 | 18.34 |
| ATOM | 2396 | CB | LYS | C | 78 | 49.017 | 15.288 | 38.533 | 1.00 | 21.80 |
| ATOM | 2397 | CG | LYS | C | 78 | 50.492 | 15.453 | 38.249 | 1.00 | 26.26 |
| ATOM | 2398 | CD | LYS | C | 78 | 50.799 | 16.212 | 36.977 | 1.00 | 33.33 |
| ATOM | 2399 | CE | LYS | C | 78 | 51.977 | 17.190 | 37.154 | 1.00 | 36.36 |
| ATOM | 2400 | NZ | LYS | C | 78 | 51.538 | 18.516 | 37.592 | 1.00 | 40.57 |
| ATOM | 2401 | N | LEU | C | 79 | 46.160 | 14.358 | 38.937 | 1.00 | 17.71 |
| ATOM | 2402 | CA | LEU | C | 79 | 45.282 | 13.528 | 39.739 | 1.00 | 19.39 |
| ATOM | 2403 | C | LEU | C | 79 | 44.465 | 12.641 | 38.836 | 1.00 | 19.34 |
| ATOM | 2404 | O | LEU | C | 79 | 44.358 | 11.479 | 39.161 | 1.00 | 22.92 |
| ATOM | 2405 | CB | LEU | C | 79 | 44.412 | 14.342 | 40.708 | 1.00 | 15.20 |
| ATOM | 2406 | CG | LEU | C | 79 | 45.179 | 15.238 | 41.695 | 1.00 | 14.54 |

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FIGURE 8A-52

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2467 | CB | VAL | C | 87 | 40.167 | 3.478 | 36.302 | 1.00 | 36.61 | C |
| ATOM | 2468 | CG1 | VAL | C | 87 | 39.054 | 2.945 | 35.450 | 1.00 | 37.46 | C |
| ATOM | 2469 | CG2 | VAL | C | 87 | 39.592 | 4.584 | 37.139 | 1.00 | 35.39 | C |
| ATOM | 2470 | N | GLU | C | 88 | 42.356 | 1.329 | 35.613 | 1.00 | 45.33 | N |
| ATOM | 2471 | CA | GLU | C | 88 | 42.933 | 0.237 | 34.842 | 1.00 | 50.04 | C |
| ATOM | 2472 | C | GLU | C | 88 | 43.480 | -0.856 | 35.761 | 1.00 | 52.28 | C |
| ATOM | 2473 | O | GLU | C | 88 | 43.503 | -2.015 | 35.374 | 1.00 | 53.46 | C |
| ATOM | 2474 | CB | GLU | C | 88 | 44.048 | 0.728 | 33.869 | 1.00 | 52.22 | O |
| ATOM | 2475 | CG | GLU | C | 88 | 43.776 | 1.785 | 32.749 | 1.00 | 56.99 | C |
| ATOM | 2476 | CD | GLU | C | 88 | 42.784 | 1.451 | 31.610 | 1.00 | 62.14 | C |
| ATOM | 2477 | OE1 | GLU | C | 88 | 42.853 | 0.348 | 31.046 | 1.00 | 66.19 | O |
| ATOM | 2478 | OE2 | GLU | C | 88 | 41.926 | 2.286 | 31.266 | 1.00 | 62.89 | O |
| ATOM | 2479 | N | CYS | C | 89 | 43.930 | -0.535 | 36.982 | 1.00 | 55.77 | N |
| ATOM | 2480 | CA | CYS | C | 89 | 44.471 | -1.508 | 37.936 | 1.00 | 58.72 | C |
| ATOM | 2481 | C | CYS | C | 89 | 43.372 | -2.333 | 38.578 | 1.00 | 60.22 | C |
| ATOM | 2482 | O | CYS | C | 89 | 43.624 | -3.464 | 39.000 | 1.00 | 61.13 | C |
| ATOM | 2483 | CB | CYS | C | 89 | 45.285 | -0.819 | 39.048 | 1.00 | 59.69 | O |
| ATOM | 2484 | SG | CYS | C | 89 | 46.103 | -1.924 | 40.239 | 1.00 | 65.48 | C |
| ATOM | 2485 | N | VAL | C | 90 | 42.159 | -1.749 | 38.657 | 1.00 | 61.71 | S |
| ATOM | 2486 | CA | VAL | C | 90 | 40.963 | -2.396 | 39.210 | 1.00 | 62.70 | N |
| ATOM | 2487 | C | VAL | C | 90 | 40.453 | -3.516 | 38.278 | 1.00 | 64.64 | C |
| ATOM | 2488 | O | VAL | C | 90 | 40.010 | -4.562 | 38.779 | 1.00 | 65.07 | C |
| ATOM | 2489 | CB | VAL | C | 90 | 39.934 | -1.260 | 39.622 | 1.00 | 60.49 | O |
| ATOM | 2490 | CG1 | VAL | C | 90 | 38.477 | -1.428 | 39.231 | 1.00 | 58.30 | C |
| ATOM | 2491 | CG2 | VAL | C | 90 | 40.023 | -1.060 | 41.125 | 1.00 | 58.40 | C |
| ATOM | 2492 | N | LYS | C | 91 | 40.591 | -3.348 | 36.938 | 1.00 | 66.41 | C |
| ATOM | 2493 | CA | LYS | C | 91 | 40.281 | -4.402 | 35.971 | 1.00 | 68.79 | N |
| ATOM | 2494 | C | LYS | C | 91 | 41.219 | -5.638 | 36.092 | 1.00 | 70.22 | C |
| ATOM | 2495 | O | LYS | C | 91 | 40.715 | -6.728 | 36.404 | 1.00 | 72.46 | C |
| ATOM | 2496 | CB | LYS | C | 91 | 40.233 | -3.836 | 34.530 | 1.00 | 68.55 | O |
| ATOM | 2497 | CG | LYS | C | 91 | 39.560 | -4.821 | 33.535 | 1.00 | 71.09 | C |
| ATOM | 2498 | CD | LYS | C | 91 | 39.779 | -4.534 | 32.028 | 1.00 | 71.78 | C |
| ATOM | 2499 | CE | LYS | C | 91 | 39.128 | -3.245 | 31.514 | 1.00 | 70.74 | C |
| ATOM | 2500 | NZ | LYS | C | 91 | 39.730 | -2.834 | 30.259 | 1.00 | 70.64 | C |
| ATOM | 2501 | N | SER | C | 104 | 25.399 | 2.470 | 38.962 | 1.00 | 56.13 | N |
| ATOM | 2502 | CA | SER | C | 104 | 25.444 | 3.921 | 38.739 | 1.00 | 55.65 | N |
| ATOM | 2503 | C | SER | C | 104 | 24.850 | 4.688 | 39.939 | 1.00 | 52.95 | C |
| ATOM | 2504 | O | SER | C | 104 | 23.647 | 4.968 | 39.947 | 1.00 | 53.89 | C |
| ATOM | 2505 | CB | SER | C | 104 | 24.797 | 4.326 | 37.337 | 1.00 | 57.16 | O |
| ATOM | 2506 | OG | SER | C | 104 | 23.517 | 3.792 | 36.940 | 1.00 | 56.67 | C |
| ATOM | 2507 | N | PRO | C | 105 | 25.618 | 5.024 | 41.000 | 1.00 | 49.29 | N |
| ATOM | 2508 | CA | PRO | C | 105 | 25.119 | 5.676 | 42.224 | 1.00 | 46.42 | N |
| ATOM | 2509 | C | PRO | C | 105 | 24.631 | 7.146 | 42.171 | 1.00 | 44.43 | C |
| ATOM | 2510 | O | PRO | C | 105 | 24.768 | 7.791 | 41.134 | 1.00 | 42.75 | C |
| ATOM | 2511 | CB | PRO | C | 105 | 26.265 | 5.445 | 43.181 | 1.00 | 45.66 | O |
| ATOM | 2512 | CG | PRO | C | 105 | 27.467 | 5.523 | 42.277 | 1.00 | 46.43 | C |
| ATOM | 2513 | CD | PRO | C | 105 | 27.036 | 4.706 | 41.089 | 1.00 | 47.56 | C |
| ATOM | 2514 | N | GLU | C | 106 | 24.023 | 7.707 | 43.240 | 1.00 | 44.38 | C |
| ATOM | 2515 | CA | GLU | C | 106 | 23.436 | 9.055 | 43.238 | 1.00 | 43.85 | N |
| ATOM | 2516 | C | GLU | C | 106 | 24.414 | 10.202 | 43.420 | 1.00 | 42.61 | C |
| ATOM | 2517 | O | GLU | C | 106 | 25.293 | 10.113 | 44.289 | 1.00 | 42.69 | C |
| ATOM | 2518 | CB | GLU | C | 106 | 22.321 | 9.281 | 44.289 | 1.00 | 45.50 | O |
| ATOM | 2519 | CG | GLU | C | 106 | 20.936 | 8.664 | 44.035 | 1.00 | 46.22 | C |
| ATOM | 2520 | CD | GLU | C | 106 | 20.404 | 8.761 | 42.607 | 1.00 | 45.82 | C |
| ATOM | 2521 | OE1 | GLU | C | 106 | 20.257 | 9.861 | 42.067 | 1.00 | 41.34 | C |
| ATOM | 2522 | OE2 | GLU | C | 106 | 20.152 | 7.699 | 42.032 | 1.00 | 48.83 | O |
| ATOM | 2523 | N | PRO | C | 107 | 24.254 | 11.291 | 42.632 | 1.00 | 41.36 | N |
| ATOM | 2524 | CA | PRO | C | 107 | 25.096 | 12.486 | 42.637 | 1.00 | 39.50 | C |
| ATOM | 2525 | C | PRO | C | 107 | 24.873 | 13.318 | 43.850 | 1.00 | 38.28 | C |
| ATOM | 2526 | O | PRO | C | 107 | 23.767 | 13.685 | 44.226 | 1.00 | 39.34 | C |

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FIGURE 8A-54

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2587 | CB | GLU | C | 114 | 33.470 | 17.344 | 51.622 | 1.00 | 26.84 | C |
| ATOM | 2588 | CG | GLU | C | 114 | 32.974 | 18.114 | 52.849 | 1.00 | 31.67 | C |
| ATOM | 2589 | CD | GLU | C | 114 | 31.578 | 18.736 | 52.701 | 1.00 | 37.47 | C |
| ATOM | 2590 | OE1 | GLU | C | 114 | 30.884 | 18.533 | 51.681 | 1.00 | 35.31 | O |
| ATOM | 2591 | OE2 | GLU | C | 114 | 31.202 | 19.468 | 53.633 | 1.00 | 40.13 | O |
| ATOM | 2592 | N | PHE | C | 115 | 35.320 | 16.775 | 49.143 | 1.00 | 20.03 | N |
| ATOM | 2593 | CA | PHE | C | 115 | 35.606 | 15.979 | 47.971 | 1.00 | 18.15 | C |
| ATOM | 2594 | C | PHE | C | 115 | 36.997 | 15.397 | 48.157 | 1.00 | 17.33 | C |
| ATOM | 2595 | O | PHE | C | 115 | 37.214 | 14.205 | 48.013 | 1.00 | 18.05 | O |
| ATOM | 2596 | CB | PHE | C | 115 | 35.524 | 16.833 | 46.705 | 1.00 | 15.90 | C |
| ATOM | 2597 | CG | PHE | C | 115 | 35.825 | 16.063 | 45.429 | 1.00 | 17.09 | C |
| ATOM | 2598 | CD1 | PHE | C | 115 | 34.861 | 15.299 | 44.845 | 1.00 | 16.21 | C |
| ATOM | 2599 | CD2 | PHE | C | 115 | 37.094 | 16.093 | 44.890 | 1.00 | 18.64 | C |
| ATOM | 2600 | CE1 | PHE | C | 115 | 35.193 | 14.558 | 43.744 | 1.00 | 19.14 | C |
| ATOM | 2601 | CE2 | PHE | C | 115 | 37.425 | 15.336 | 43.795 | 1.00 | 18.76 | C |
| ATOM | 2602 | CZ | PHE | C | 115 | 36.463 | 14.570 | 43.217 | 1.00 | 19.41 | C |
| ATOM | 2603 | N | PHE | C | 116 | 38.010 | 16.167 | 48.509 | 1.00 | 19.36 | N |
| ATOM | 2604 | CA | PHE | C | 116 | 39.361 | 15.618 | 48.454 | 1.00 | 17.90 | C |
| ATOM | 2605 | C | PHE | C | 116 | 39.621 | 14.678 | 49.623 | 1.00 | 18.24 | C |
| ATOM | 2606 | O | PHE | C | 116 | 40.505 | 13.855 | 49.549 | 1.00 | 19.98 | O |
| ATOM | 2607 | CB | PHE | C | 116 | 40.376 | 16.744 | 48.162 | 1.00 | 16.33 | C |
| ATOM | 2608 | CG | PHE | C | 116 | 40.442 | 17.170 | 46.679 | 1.00 | 15.27 | C |
| ATOM | 2609 | CD1 | PHE | C | 116 | 41.052 | 16.328 | 45.753 | 1.00 | 14.80 | C |
| ATOM | 2610 | CD2 | PHE | C | 116 | 39.806 | 18.324 | 46.240 | 1.00 | 12.85 | C |
| ATOM | 2611 | CE1 | PHE | C | 116 | 40.967 | 16.602 | 44.409 | 1.00 | 12.34 | C |
| ATOM | 2612 | CE2 | PHE | C | 116 | 39.715 | 18.569 | 44.885 | 1.00 | 14.12 | C |
| ATOM | 2613 | CZ | PHE | C | 116 | 40.289 | 17.711 | 43.980 | 1.00 | 10.60 | C |
| ATOM | 2614 | N | ARG | C | 117 | 38.755 | 14.664 | 50.641 | 1.00 | 20.78 | N |
| ATOM | 2615 | CA | ARG | C | 117 | 38.796 | 13.751 | 51.770 | 1.00 | 21.33 | C |
| ATOM | 2616 | C | ARG | C | 117 | 38.412 | 12.368 | 51.308 | 1.00 | 20.46 | C |
| ATOM | 2617 | O | ARG | C | 117 | 39.076 | 11.405 | 51.639 | 1.00 | 21.70 | O |
| ATOM | 2618 | CB | ARG | C | 117 | 37.823 | 14.244 | 52.840 | 1.00 | 21.70 | C |
| ATOM | 2619 | CG | ARG | C | 117 | 37.838 | 13.513 | 54.177 | 1.00 | 27.63 | C |
| ATOM | 2620 | CD | ARG | C | 117 | 36.826 | 14.115 | 55.165 | 1.00 | 29.36 | C |
| ATOM | 2621 | NE | ARG | C | 117 | 37.230 | 15.464 | 55.616 | 1.00 | 32.11 | N |
| ATOM | 2622 | CZ | ARG | C | 117 | 36.411 | 16.535 | 55.565 | 1.00 | 32.37 | C |
| ATOM | 2623 | NH1 | ARG | C | 117 | 35.179 | 16.464 | 55.047 | 1.00 | 32.61 | N |
| ATOM | 2624 | NH2 | ARG | C | 117 | 36.836 | 17.701 | 56.025 | 1.00 | 30.98 | N |
| ATOM | 2625 | N | ILE | C | 118 | 37.342 | 12.263 | 50.540 | 1.00 | 21.91 | N |
| ATOM | 2626 | CA | ILE | C | 118 | 36.897 | 11.031 | 49.882 | 1.00 | 22.55 | C |
| ATOM | 2627 | C | ILE | C | 118 | 37.944 | 10.504 | 48.890 | 1.00 | 23.60 | C |
| ATOM | 2628 | O | ILE | C | 118 | 38.254 | 9.316 | 48.853 | 1.00 | 24.72 | O |
| ATOM | 2629 | CB | ILE | C | 118 | 35.527 | 11.358 | 49.213 | 1.00 | 22.47 | C |
| ATOM | 2630 | CG1 | ILE | C | 118 | 34.467 | 11.506 | 50.293 | 1.00 | 21.67 | C |
| ATOM | 2631 | CG2 | ILE | C | 118 | 35.117 | 10.338 | 48.161 | 1.00 | 21.48 | C |
| ATOM | 2632 | CD1 | ILE | C | 118 | 33.164 | 12.169 | 49.825 | 1.00 | 21.12 | C |
| ATOM | 2633 | N | PHE | C | 119 | 38.544 | 11.402 | 48.103 | 1.00 | 23.86 | N |
| ATOM | 2634 | CA | PHE | C | 119 | 39.633 | 11.098 | 47.186 | 1.00 | 22.73 | C |
| ATOM | 2635 | C | PHE | C | 119 | 40.816 | 10.488 | 47.916 | 1.00 | 24.24 | C |
| ATOM | 2636 | O | PHE | C | 119 | 41.233 | 9.416 | 47.511 | 1.00 | 24.28 | O |
| ATOM | 2637 | CB | PHE | C | 119 | 40.038 | 12.357 | 46.426 | 1.00 | 15.88 | C |
| ATOM | 2638 | CG | PHE | C | 119 | 41.297 | 12.224 | 45.624 | 1.00 | 15.30 | C |
| ATOM | 2639 | CD1 | PHE | C | 119 | 41.231 | 11.724 | 44.354 | 1.00 | 15.03 | C |
| ATOM | 2640 | CD2 | PHE | C | 119 | 42.495 | 12.639 | 46.172 | 1.00 | 12.85 | C |
| ATOM | 2641 | CE1 | PHE | C | 119 | 42.412 | 11.623 | 43.653 | 1.00 | 15.97 | C |
| ATOM | 2642 | CE2 | PHE | C | 119 | 43.675 | 12.526 | 45.473 | 1.00 | 15.16 | C |
| ATOM | 2643 | CZ | PHE | C | 119 | 43.630 | 12.003 | 44.206 | 1.00 | 16.33 | C |
| ATOM | 2644 | N | ASN | C | 120 | 41.396 | 11.145 | 48.936 | 1.00 | 26.61 | N |
| ATOM | 2645 | CA | ASN | C | 120 | 42.511 | 10.621 | 49.728 | 1.00 | 27.10 | C |
| ATOM | 2646 | C | ASN | C | 120 | 42.225 | 9.301 | 50.400 | 1.00 | 28.31 | C |

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FIGURE 8A-55

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2647 | O | ASN | C | 120 | 43.081 | 8.433 | 50.376 | 1.00 | 28.63 | O |
| ATOM | 2648 | CB | ASN | C | 120 | 42.959 | 11.590 | 50.783 | 1.00 | 24.50 | C |
| ATOM | 2649 | CG | ASN | C | 120 | 43.837 | 12.659 | 50.215 | 1.00 | 27.34 | O |
| ATOM | 2650 | OD1 | ASN | C | 120 | 43.864 | 13.757 | 50.761 | 1.00 | 32.26 | C |
| ATOM | 2651 | ND2 | ASN | C | 120 | 44.628 | 12.420 | 49.169 | 1.00 | 29.64 | O |
| ATOM | 2652 | N | ARG | C | 121 | 41.017 | 9.136 | 50.947 | 1.00 | 30.80 | N |
| ATOM | 2653 | CA | ARG | C | 121 | 40.549 | 7.862 | 51.441 | 1.00 | 35.49 | C |
| ATOM | 2654 | C | ARG | C | 121 | 40.514 | 6.767 | 50.357 | 1.00 | 36.43 | C |
| ATOM | 2655 | O | ARG | C | 121 | 40.859 | 5.616 | 50.628 | 1.00 | 38.58 | O |
| ATOM | 2656 | CB | ARG | C | 121 | 39.202 | 8.108 | 52.138 | 1.00 | 37.63 | C |
| ATOM | 2657 | CG | ARG | C | 121 | 38.534 | 6.865 | 52.651 | 1.00 | 42.24 | C |
| ATOM | 2658 | CD | ARG | C | 121 | 37.240 | 7.194 | 53.373 | 1.00 | 47.82 | C |
| ATOM | 2659 | NE | ARG | C | 121 | 36.399 | 6.001 | 53.529 | 1.00 | 51.79 | C |
| ATOM | 2660 | CZ | ARG | C | 121 | 36.788 | 4.912 | 54.233 | 1.00 | 55.38 | N |
| ATOM | 2661 | NH1 | ARG | C | 121 | 38.016 | 4.799 | 54.783 | 1.00 | 57.12 | N |
| ATOM | 2662 | NH2 | ARG | C | 121 | 35.928 | 3.904 | 54.446 | 1.00 | 55.34 | N |
| ATOM | 2663 | N | SER | C | 122 | 40.171 | 7.089 | 49.106 | 1.00 | 36.49 | N |
| ATOM | 2664 | CA | SER | C | 122 | 40.274 | 6.177 | 47.974 | 1.00 | 36.44 | C |
| ATOM | 2665 | C | SER | C | 122 | 41.660 | 5.723 | 47.529 | 1.00 | 37.85 | C |
| ATOM | 2666 | O | SER | C | 122 | 41.874 | 4.556 | 47.235 | 1.00 | 39.23 | O |
| ATOM | 2667 | CB | SER | C | 122 | 39.613 | 6.814 | 46.788 | 1.00 | 34.58 | O |
| ATOM | 2668 | OG | SER | C | 122 | 38.286 | 7.132 | 47.155 | 1.00 | 34.47 | O |
| ATOM | 2669 | N | ILE | C | 123 | 42.638 | 6.599 | 47.409 | 1.00 | 38.85 | N |
| ATOM | 2670 | CA | ILE | C | 123 | 43.949 | 6.180 | 46.985 | 1.00 | 43.11 | C |
| ATOM | 2671 | C | ILE | C | 123 | 44.589 | 5.456 | 48.157 | 1.00 | 46.18 | C |
| ATOM | 2672 | O | ILE | C | 123 | 45.449 | 4.614 | 47.937 | 1.00 | 47.69 | O |
| ATOM | 2673 | CB | ILE | C | 123 | 44.843 | 7.378 | 46.505 | 1.00 | 42.65 | C |
| ATOM | 2674 | CG1 | ILE | C | 123 | 44.147 | 8.410 | 45.599 | 1.00 | 38.38 | C |
| ATOM | 2675 | CG2 | ILE | C | 123 | 46.146 | 6.866 | 45.872 | 1.00 | 43.09 | C |
| ATOM | 2676 | CD1 | ILE | C | 123 | 43.242 | 7.872 | 44.489 | 1.00 | 35.80 | C |
| ATOM | 2677 | N | ASP | C | 124 | 44.206 | 5.755 | 49.402 | 1.00 | 50.61 | N |
| ATOM | 2678 | CA | ASP | C | 124 | 44.805 | 5.095 | 50.564 | 1.00 | 54.85 | C |
| ATOM | 2679 | C | ASP | C | 124 | 44.197 | 3.730 | 50.882 | 1.00 | 54.20 | C |
| ATOM | 2680 | O | ASP | C | 124 | 44.774 | 2.898 | 51.586 | 1.00 | 54.57 | O |
| ATOM | 2681 | CB | ASP | C | 124 | 44.788 | 5.989 | 51.823 | 1.00 | 59.47 | C |
| ATOM | 2682 | CG | ASP | C | 124 | 45.794 | 7.151 | 51.915 | 1.00 | 63.36 | C |
| ATOM | 2683 | OD1 | ASP | C | 124 | 45.935 | 7.919 | 50.949 | 1.00 | 63.45 | O |
| ATOM | 2684 | OD2 | ASP | C | 124 | 46.414 | 7.295 | 52.988 | 1.00 | 66.94 | O |
| ATOM | 2685 | N | ALA | C | 125 | 43.039 | 3.460 | 50.281 | 1.00 | 54.57 | N |
| ATOM | 2686 | CA | ALA | C | 125 | 42.427 | 2.137 | 50.314 | 1.00 | 56.99 | C |
| ATOM | 2687 | C | ALA | C | 125 | 43.150 | 1.108 | 49.440 | 1.00 | 58.85 | C |
| ATOM | 2688 | O | ALA | C | 125 | 42.617 | 0.022 | 49.161 | 1.00 | 59.46 | O |
| ATOM | 2689 | CB | ALA | C | 125 | 40.982 | 2.263 | 49.824 | 1.00 | 56.08 | C |
| ATOM | 2690 | N | PHE | C | 126 | 44.343 | 1.552 | 48.975 | 1.00 | 60.81 | N |
| ATOM | 2691 | CA | PHE | C | 126 | 45.408 | 0.793 | 48.316 | 1.00 | 62.82 | C |
| ATOM | 2692 | C | PHE | C | 126 | 46.675 | 0.603 | 49.241 | 1.00 | 64.91 | C |
| ATOM | 2693 | O | PHE | C | 126 | 47.801 | 0.492 | 48.731 | 1.00 | 65.88 | O |
| ATOM | 2694 | CB | PHE | C | 126 | 45.715 | 1.476 | 46.898 | 1.00 | 60.15 | C |
| ATOM | 2695 | CG | PHE | C | 126 | 44.638 | 1.419 | 45.778 | 1.00 | 57.55 | C |
| ATOM | 2696 | CD1 | PHE | C | 126 | 43.594 | 2.334 | 45.731 | 1.00 | 56.09 | C |
| ATOM | 2697 | CD2 | PHE | C | 126 | 44.655 | 0.421 | 44.813 | 1.00 | 56.90 | C |
| ATOM | 2698 | CE1 | PHE | C | 126 | 42.568 | 2.227 | 44.807 | 1.00 | 52.24 | C |
| ATOM | 2699 | CE2 | PHE | C | 126 | 43.627 | 0.319 | 43.884 | 1.00 | 54.42 | C |
| ATOM | 2700 | CZ | PHE | C | 126 | 42.573 | 1.208 | 43.889 | 1.00 | 52.99 | C |
| TER | 2702 | | PHE | C | 126 | | | | | | |
| ATOM | 2703 | N | ASN | D | 11 | 47.774 | 44.287 | 38.626 | 1.00 | 52.77 | N |
| ATOM | 2704 | CA | ASN | D | 11 | 46.416 | 43.904 | 38.273 | 1.00 | 53.01 | C |
| ATOM | 2705 | C | ASN | D | 11 | 46.383 | 43.039 | 36.995 | 1.00 | 52.04 | C |
| ATOM | 2706 | O | ASN | D | 11 | 46.673 | 41.852 | 37.139 | 1.00 | 53.30 | O |
| ATOM | 2707 | CB | ASN | D | 11 | 45.488 | 45.136 | 38.154 | 1.00 | 52.37 | C |

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FIGURE 8A-56

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 2708 | N | VAL | D | 12 | 46.135 | 43.551 | 35.763 | 1.00 | 49.81 | N |
| ATOM | 2709 | CA | VAL | D | 12 | 45.936 | 42.823 | 34.490 | 1.00 | 45.10 | C |
| ATOM | 2710 | C | VAL | D | 12 | 46.697 | 41.529 | 34.194 | 1.00 | 40.73 | O |
| ATOM | 2711 | O | VAL | D | 12 | 46.109 | 40.477 | 33.958 | 1.00 | 39.20 | C |
| ATOM | 2712 | CB | VAL | D | 12 | 46.118 | 43.863 | 33.336 | 1.00 | 46.99 | C |
| ATOM | 2713 | CG1 | VAL | D | 12 | 46.377 | 43.229 | 31.966 | 1.00 | 47.11 | C |
| ATOM | 2714 | CG2 | VAL | D | 12 | 44.888 | 44.784 | 33.225 | 1.00 | 46.26 | C |
| ATOM | 2715 | N | LYS | D | 13 | 48.014 | 41.610 | 34.165 | 1.00 | 37.97 | C |
| ATOM | 2716 | CA | LYS | D | 13 | 48.844 | 40.432 | 34.132 | 1.00 | 36.45 | C |
| ATOM | 2717 | C | LYS | D | 13 | 48.402 | 39.322 | 35.117 | 1.00 | 36.18 | C |
| ATOM | 2718 | O | LYS | D | 13 | 48.194 | 38.166 | 34.709 | 1.00 | 37.38 | C |
| ATOM | 2719 | CB | LYS | D | 13 | 50.258 | 40.905 | 34.451 | 1.00 | 35.89 | O |
| ATOM | 2720 | N | ASP | D | 14 | 48.190 | 39.643 | 36.410 | 1.00 | 33.96 | C |
| ATOM | 2721 | CA | ASP | D | 14 | 47.703 | 38.684 | 37.372 | 1.00 | 29.22 | N |
| ATOM | 2722 | C | ASP | D | 14 | 46.220 | 38.409 | 37.305 | 1.00 | 25.55 | C |
| ATOM | 2723 | O | ASP | D | 14 | 45.799 | 37.316 | 37.647 | 1.00 | 25.36 | O |
| ATOM | 2724 | CB | ASP | D | 14 | 48.158 | 39.126 | 38.725 | 1.00 | 33.71 | O |
| ATOM | 2725 | CG | ASP | D | 14 | 49.573 | 38.623 | 39.084 | 1.00 | 41.45 | O |
| ATOM | 2726 | OD1 | ASP | D | 14 | 50.178 | 37.858 | 38.316 | 1.00 | 45.64 | O |
| ATOM | 2727 | OD2 | ASP | D | 14 | 50.083 | 38.981 | 40.161 | 1.00 | 44.73 | O |
| ATOM | 2728 | N | VAL | D | 15 | 45.421 | 39.347 | 36.809 | 1.00 | 22.15 | O |
| ATOM | 2729 | CA | VAL | D | 15 | 44.000 | 39.173 | 36.672 | 1.00 | 19.73 | N |
| ATOM | 2730 | C | VAL | D | 15 | 43.683 | 38.044 | 35.731 | 1.00 | 21.56 | C |
| ATOM | 2731 | O | VAL | D | 15 | 42.825 | 37.217 | 36.016 | 1.00 | 23.37 | O |
| ATOM | 2732 | CB | VAL | D | 15 | 43.294 | 40.462 | 36.234 | 1.00 | 18.49 | C |
| ATOM | 2733 | CG1 | VAL | D | 15 | 41.883 | 40.238 | 35.684 | 1.00 | 17.31 | C |
| ATOM | 2734 | CG2 | VAL | D | 15 | 43.093 | 41.327 | 37.450 | 1.00 | 17.77 | C |
| ATOM | 2735 | N | THR | D | 16 | 44.387 | 37.974 | 34.623 | 1.00 | 22.81 | N |
| ATOM | 2736 | CA | THR | D | 16 | 44.166 | 36.943 | 33.605 | 1.00 | 24.47 | C |
| ATOM | 2737 | C | THR | D | 16 | 44.517 | 35.513 | 34.082 | 1.00 | 21.91 | C |
| ATOM | 2738 | O | THR | D | 16 | 43.904 | 34.526 | 33.676 | 1.00 | 20.78 | O |
| ATOM | 2739 | CB | THR | D | 16 | 44.991 | 37.520 | 32.381 | 1.00 | 26.36 | C |
| ATOM | 2740 | OG1 | THR | D | 16 | 44.076 | 38.310 | 31.630 | 1.00 | 28.31 | C |
| ATOM | 2741 | CG2 | THR | D | 16 | 45.721 | 36.529 | 31.530 | 1.00 | 28.93 | C |
| ATOM | 2742 | N | LYS | D | 17 | 45.470 | 35.415 | 35.016 | 1.00 | 20.72 | N |
| ATOM | 2743 | CA | LYS | D | 17 | 45.958 | 34.179 | 35.596 | 1.00 | 20.21 | C |
| ATOM | 2744 | C | LYS | D | 17 | 45.019 | 33.719 | 36.683 | 1.00 | 18.63 | C |
| ATOM | 2745 | O | LYS | D | 17 | 44.754 | 32.526 | 36.783 | 1.00 | 21.04 | O |
| ATOM | 2746 | CB | LYS | D | 17 | 47.277 | 34.522 | 36.207 | 1.00 | 24.75 | C |
| ATOM | 2747 | CG | LYS | D | 17 | 48.163 | 33.373 | 36.590 | 1.00 | 29.44 | C |
| ATOM | 2748 | CD | LYS | D | 17 | 49.365 | 33.928 | 37.347 | 1.00 | 32.96 | C |
| ATOM | 2749 | CE | LYS | D | 17 | 50.423 | 34.474 | 36.422 | 1.00 | 36.20 | C |
| ATOM | 2750 | NZ | LYS | D | 17 | 51.313 | 35.272 | 37.230 | 1.00 | 39.87 | N |
| ATOM | 2751 | N | LEU | D | 18 | 44.483 | 34.656 | 37.468 | 1.00 | 16.11 | C |
| ATOM | 2752 | CA | LEU | D | 18 | 43.391 | 34.389 | 38.362 | 1.00 | 13.77 | C |
| ATOM | 2753 | C | LEU | D | 18 | 42.158 | 33.926 | 37.636 | 1.00 | 14.10 | C |
| ATOM | 2754 | O | LEU | D | 18 | 41.662 | 32.898 | 38.072 | 1.00 | 17.61 | O |
| ATOM | 2755 | CB | LEU | D | 18 | 43.070 | 35.599 | 39.180 | 1.00 | 14.87 | C |
| ATOM | 2756 | CG | LEU | D | 18 | 42.103 | 35.485 | 40.362 | 1.00 | 15.58 | C |
| ATOM | 2757 | CD1 | LEU | D | 18 | 42.567 | 34.568 | 41.470 | 1.00 | 11.31 | C |
| ATOM | 2758 | CD2 | LEU | D | 18 | 41.872 | 36.849 | 40.952 | 1.00 | 15.28 | C |
| ATOM | 2759 | N | VAL | D | 19 | 41.617 | 34.544 | 36.561 | 1.00 | 15.42 | N |
| ATOM | 2760 | CA | VAL | D | 19 | 40.479 | 34.034 | 35.786 | 1.00 | 13.39 | C |
| ATOM | 2761 | C | VAL | D | 19 | 40.704 | 32.587 | 35.385 | 1.00 | 14.30 | C |
| ATOM | 2762 | O | VAL | D | 19 | 39.824 | 31.744 | 35.542 | 1.00 | 13.93 | O |
| ATOM | 2763 | CB | VAL | D | 19 | 40.251 | 34.838 | 34.489 | 1.00 | 14.39 | C |
| ATOM | 2764 | CG1 | VAL | D | 19 | 39.059 | 34.330 | 33.694 | 1.00 | 11.41 | C |
| ATOM | 2765 | CG2 | VAL | D | 19 | 39.913 | 36.255 | 34.797 | 1.00 | 12.80 | C |
| ATOM | 2766 | N | ALA | D | 20 | 41.911 | 32.288 | 34.876 | 1.00 | 14.50 | C |
| ATOM | 2767 | CA | ALA | D | 20 | 42.319 | 30.924 | 34.543 | 1.00 | 15.90 | N |

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FIGURE 8A-57

| | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2768 | C | ALA | D | 20 | 42.340 | 29.894 | 35.680 | 1.00 | 16.27 |
| ATOM | 2769 | O | ALA | D | 20 | 42.153 | 28.697 | 35.464 | 1.00 | 14.91 |
| ATOM | 2770 | CB | ALA | D | 20 | 43.719 | 30.983 | 33.946 | 1.00 | 16.48 |
| ATOM | 2771 | N | ASN | D | 21 | 42.543 | 30.396 | 36.914 | 1.00 | 16.20 |
| ATOM | 2772 | CA | ASN | D | 21 | 42.665 | 29.549 | 38.081 | 1.00 | 14.59 |
| ATOM | 2773 | C | ASN | D | 21 | 41.408 | 29.513 | 38.923 | 1.00 | 15.22 |
| ATOM | 2774 | O | ASN | D | 21 | 41.343 | 28.894 | 39.982 | 1.00 | 14.76 |
| ATOM | 2775 | CB | ASN | D | 21 | 43.863 | 30.085 | 38.853 | 1.00 | 15.31 |
| ATOM | 2776 | CG | ASN | D | 21 | 44.760 | 29.000 | 39.360 | 1.00 | 15.31 |
| ATOM | 2777 | OD1 | ASN | D | 21 | 45.002 | 28.023 | 38.659 | 1.00 | 12.22 |
| ATOM | 2778 | ND2 | ASN | D | 21 | 45.313 | 29.122 | 40.545 | 1.00 | 15.31 |
| ATOM | 2779 | N | LEU | D | 22 | 40.364 | 30.201 | 38.493 | 1.00 | 14.81 |
| ATOM | 2780 | CA | LEU | D | 22 | 39.069 | 30.126 | 39.157 | 1.00 | 15.32 |
| ATOM | 2781 | C | LEU | D | 22 | 38.172 | 29.241 | 38.319 | 1.00 | 15.81 |
| ATOM | 2782 | O | LEU | D | 22 | 38.337 | 29.289 | 37.109 | 1.00 | 18.22 |
| ATOM | 2783 | CB | LEU | D | 22 | 38.470 | 31.498 | 39.326 | 1.00 | 11.04 |
| ATOM | 2784 | CG | LEU | D | 22 | 39.203 | 32.454 | 40.210 | 1.00 | 10.12 |
| ATOM | 2785 | CD1 | LEU | D | 22 | 38.580 | 33.801 | 40.004 | 1.00 | 11.85 |
| ATOM | 2786 | CD2 | LEU | D | 22 | 39.108 | 32.071 | 41.671 | 1.00 | 10.74 |
| ATOM | 2787 | N | PRO | D | 23 | 37.246 | 28.422 | 38.825 | 1.00 | 16.11 |
| ATOM | 2788 | CA | PRO | D | 23 | 36.365 | 27.588 | 38.004 | 1.00 | 15.30 |
| ATOM | 2789 | C | PRO | D | 23 | 35.533 | 28.456 | 37.064 | 1.00 | 16.55 |
| ATOM | 2790 | O | PRO | D | 23 | 35.044 | 29.485 | 37.502 | 1.00 | 18.78 |
| ATOM | 2791 | CB | PRO | D | 23 | 35.474 | 26.944 | 39.027 | 1.00 | 14.03 |
| ATOM | 2792 | CG | PRO | D | 23 | 36.252 | 27.043 | 40.317 | 1.00 | 16.22 |
| ATOM | 2793 | CD | PRO | D | 23 | 36.854 | 28.409 | 40.228 | 1.00 | 15.04 |
| ATOM | 2794 | N | LYS | D | 24 | 35.319 | 28.105 | 35.785 | 1.00 | 19.22 |
| ATOM | 2795 | CA | LYS | D | 24 | 34.492 | 28.864 | 34.822 | 1.00 | 19.57 |
| ATOM | 2796 | C | LYS | D | 24 | 33.027 | 28.975 | 35.241 | 1.00 | 18.94 |
| ATOM | 2797 | O | LYS | D | 24 | 32.381 | 29.956 | 34.910 | 1.00 | 22.65 |
| ATOM | 2798 | CB | LYS | D | 24 | 34.575 | 28.214 | 33.425 | 1.00 | 20.25 |
| ATOM | 2799 | CG | LYS | D | 24 | 35.853 | 28.425 | 32.655 | 1.00 | 19.83 |
| ATOM | 2800 | CD | LYS | D | 24 | 36.049 | 27.261 | 31.683 | 1.00 | 20.33 |
| ATOM | 2801 | CE | LYS | D | 24 | 37.542 | 27.297 | 31.291 | 1.00 | 25.04 |
| ATOM | 2802 | NZ | LYS | D | 24 | 38.019 | 26.084 | 30.623 | 1.00 | 27.36 |
| ATOM | 2803 | N | ASP | D | 25 | 32.490 | 28.011 | 36.007 | 1.00 | 20.97 |
| ATOM | 2804 | CA | ASP | D | 25 | 31.146 | 27.984 | 36.585 | 1.00 | 20.24 |
| ATOM | 2805 | C | ASP | D | 25 | 31.084 | 28.420 | 38.037 | 1.00 | 20.26 |
| ATOM | 2806 | O | ASP | D | 25 | 30.092 | 28.177 | 38.714 | 1.00 | 24.64 |
| ATOM | 2807 | CB | ASP | D | 25 | 30.557 | 26.555 | 36.502 | 1.00 | 21.95 |
| ATOM | 2808 | CG | ASP | D | 25 | 31.274 | 25.501 | 37.333 | 1.00 | 26.54 |
| ATOM | 2809 | OD1 | ASP | D | 25 | 32.429 | 25.721 | 37.693 | 1.00 | 28.24 |
| ATOM | 2810 | OD2 | ASP | D | 25 | 30.697 | 24.445 | 37.616 | 1.00 | 29.75 |
| ATOM | 2811 | N | TYR | D | 26 | 32.109 | 29.038 | 38.591 | 1.00 | 19.65 |
| ATOM | 2812 | CA | TYR | D | 26 | 31.978 | 29.716 | 39.865 | 1.00 | 19.99 |
| ATOM | 2813 | C | TYR | D | 26 | 31.327 | 31.078 | 39.666 | 1.00 | 20.55 |
| ATOM | 2814 | O | TYR | D | 26 | 31.837 | 31.882 | 38.892 | 1.00 | 23.24 |
| ATOM | 2815 | CB | TYR | D | 26 | 33.388 | 29.886 | 40.446 | 1.00 | 18.93 |
| ATOM | 2816 | CG | TYR | D | 26 | 33.487 | 30.459 | 41.844 | 1.00 | 18.30 |
| ATOM | 2817 | CD1 | TYR | D | 26 | 32.718 | 29.938 | 42.855 | 1.00 | 17.48 |
| ATOM | 2818 | CD2 | TYR | D | 26 | 34.309 | 31.538 | 42.057 | 1.00 | 19.75 |
| ATOM | 2819 | CE1 | TYR | D | 26 | 32.689 | 30.542 | 44.078 | 1.00 | 17.10 |
| ATOM | 2820 | CE2 | TYR | D | 26 | 34.304 | 32.124 | 43.291 | 1.00 | 21.03 |
| ATOM | 2821 | CZ | TYR | D | 26 | 33.494 | 31.613 | 44.276 | 1.00 | 19.84 |
| ATOM | 2822 | OH | TYR | D | 26 | 33.553 | 32.163 | 45.538 | 1.00 | 26.79 |
| HETATM | 2823 | N | MSE | D | 27 | 30.240 | 31.351 | 40.390 | 1.00 | 20.11 |
| HETATM | 2824 | CA | MSE | D | 27 | 29.563 | 32.640 | 40.409 | 1.00 | 19.68 |
| HETATM | 2825 | C | MSE | D | 27 | 29.972 | 33.547 | 41.554 | 1.00 | 19.24 |
| HETATM | 2826 | O | MSE | D | 27 | 29.844 | 33.217 | 42.722 | 1.00 | 18.84 |
| HETATM | 2827 | CB | MSE | D | 27 | 28.030 | 32.478 | 40.470 | 1.00 | 25.00 |

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FIGURE 8A-58

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|----|
| HETATM | 2828 | CG | MSE | D | 27 | 27.356 | 31.633 | 39.361 | 1.00 | 27.34 | C |
| HETATM | 2829 | SE | MSE | D | 27 | 28.005 | 31.953 | 37.549 | 1.00 | 33.76 | SE |
| HETATM | 2830 | CE | MSE | D | 27 | 27.146 | 33.538 | 37.334 | 1.00 | 29.16 | C |
| ATOM | 2831 | N | ILE | D | 28 | 30.503 | 34.700 | 41.191 | 1.00 | 18.26 | N |
| ATOM | 2832 | CA | ILE | D | 28 | 30.838 | 35.733 | 42.127 | 1.00 | 18.98 | C |
| ATOM | 2833 | C | ILE | D | 28 | 29.668 | 36.703 | 42.239 | 1.00 | 19.61 | O |
| ATOM | 2834 | O | ILE | D | 28 | 29.151 | 37.088 | 41.196 | 1.00 | 22.18 | C |
| ATOM | 2835 | CB | ILE | D | 28 | 32.136 | 36.421 | 41.662 | 1.00 | 15.61 | O |
| ATOM | 2836 | CG1 | ILE | D | 28 | 33.234 | 35.398 | 41.469 | 1.00 | 12.73 | C |
| ATOM | 2837 | CG2 | ILE | D | 28 | 32.593 | 37.471 | 42.693 | 1.00 | 15.00 | C |
| ATOM | 2838 | CD1 | ILE | D | 28 | 34.487 | 35.969 | 40.818 | 1.00 | 10.07 | C |
| ATOM | 2839 | N | THR | D | 29 | 29.199 | 37.105 | 43.433 | 1.00 | 20.30 | C |
| ATOM | 2840 | CA | THR | D | 29 | 28.142 | 38.118 | 43.587 | 1.00 | 18.55 | N |
| ATOM | 2841 | C | THR | D | 29 | 28.720 | 39.514 | 43.593 | 1.00 | 18.51 | C |
| ATOM | 2842 | O | THR | D | 29 | 29.681 | 39.757 | 44.305 | 1.00 | 20.24 | O |
| ATOM | 2843 | CB | THR | D | 29 | 27.248 | 37.915 | 44.853 | 1.00 | 18.42 | O |
| ATOM | 2844 | OG1 | THR | D | 29 | 26.791 | 36.570 | 44.817 | 1.00 | 20.41 | O |
| ATOM | 2845 | CG2 | THR | D | 29 | 25.982 | 38.747 | 44.836 | 1.00 | 16.39 | C |
| ATOM | 2846 | N | LEU | D | 30 | 28.205 | 40.455 | 42.785 | 1.00 | 18.52 | N |
| ATOM | 2847 | CA | LEU | D | 30 | 28.610 | 41.845 | 42.783 | 1.00 | 17.78 | C |
| ATOM | 2848 | C | LEU | D | 30 | 27.305 | 42.598 | 42.724 | 1.00 | 19.35 | C |
| ATOM | 2849 | O | LEU | D | 30 | 26.420 | 42.245 | 41.946 | 1.00 | 19.98 | C |
| ATOM | 2850 | CB | LEU | D | 30 | 29.390 | 42.149 | 41.505 | 1.00 | 18.28 | C |
| ATOM | 2851 | CG | LEU | D | 30 | 29.905 | 43.557 | 41.154 | 1.00 | 15.52 | C |
| ATOM | 2852 | CD1 | LEU | D | 30 | 30.720 | 44.170 | 42.241 | 1.00 | 15.62 | C |
| ATOM | 2853 | CD2 | LEU | D | 30 | 30.732 | 43.522 | 39.879 | 1.00 | 17.11 | C |
| ATOM | 2854 | N | LYS | D | 31 | 27.150 | 43.613 | 43.560 | 1.00 | 20.05 | C |
| ATOM | 2855 | CA | LYS | D | 31 | 26.046 | 44.522 | 43.409 | 1.00 | 21.35 | C |
| ATOM | 2856 | C | LYS | D | 31 | 26.413 | 45.564 | 42.354 | 1.00 | 23.46 | C |
| ATOM | 2857 | O | LYS | D | 31 | 27.223 | 46.470 | 42.561 | 1.00 | 23.96 | C |
| ATOM | 2858 | CB | LYS | D | 31 | 25.702 | 45.148 | 44.722 | 1.00 | 21.22 | C |
| ATOM | 2859 | CG | LYS | D | 31 | 25.353 | 44.109 | 45.766 | 1.00 | 23.53 | C |
| ATOM | 2860 | CD | LYS | D | 31 | 24.738 | 44.814 | 46.976 | 1.00 | 28.13 | C |
| ATOM | 2861 | CE | LYS | D | 31 | 24.583 | 43.890 | 48.182 | 1.00 | 29.07 | C |
| ATOM | 2862 | NZ | LYS | D | 31 | 23.982 | 44.617 | 49.293 | 1.00 | 34.24 | C |
| ATOM | 2863 | N | TYR | D | 32 | 25.818 | 45.356 | 41.172 | 1.00 | 25.01 | N |
| ATOM | 2864 | CA | TYR | D | 32 | 26.219 | 46.004 | 39.925 | 1.00 | 25.06 | N |
| ATOM | 2865 | C | TYR | D | 32 | 25.377 | 47.248 | 39.752 | 1.00 | 26.53 | C |
| ATOM | 2866 | O | TYR | D | 32 | 24.167 | 47.293 | 40.046 | 1.00 | 27.71 | C |
| ATOM | 2867 | CB | TYR | D | 32 | 26.050 | 44.978 | 38.778 | 1.00 | 25.42 | C |
| ATOM | 2868 | CG | TYR | D | 32 | 26.196 | 45.465 | 37.336 | 1.00 | 24.15 | C |
| ATOM | 2869 | CD1 | TYR | D | 32 | 27.433 | 45.460 | 36.728 | 1.00 | 22.29 | C |
| ATOM | 2870 | CD2 | TYR | D | 32 | 25.071 | 45.915 | 36.672 | 1.00 | 23.90 | C |
| ATOM | 2871 | CE1 | TYR | D | 32 | 27.558 | 45.961 | 35.459 | 1.00 | 24.06 | C |
| ATOM | 2872 | CE2 | TYR | D | 32 | 25.183 | 46.427 | 35.409 | 1.00 | 25.00 | C |
| ATOM | 2873 | CZ | TYR | D | 32 | 26.427 | 46.458 | 34.822 | 1.00 | 26.48 | C |
| ATOM | 2874 | OH | TYR | D | 32 | 26.533 | 47.012 | 33.558 | 1.00 | 26.81 | C |
| ATOM | 2875 | N | VAL | D | 33 | 26.099 | 48.297 | 39.333 | 1.00 | 28.52 | N |
| ATOM | 2876 | CA | VAL | D | 33 | 25.505 | 49.613 | 39.093 | 1.00 | 27.57 | C |
| ATOM | 2877 | C | VAL | D | 33 | 24.973 | 49.634 | 37.670 | 1.00 | 27.14 | C |
| ATOM | 2878 | O | VAL | D | 33 | 25.769 | 49.693 | 36.750 | 1.00 | 28.15 | C |
| ATOM | 2879 | CB | VAL | D | 33 | 26.529 | 50.724 | 39.288 | 1.00 | 26.82 | C |
| ATOM | 2880 | CG1 | VAL | D | 33 | 25.931 | 52.066 | 38.921 | 1.00 | 25.83 | C |
| ATOM | 2881 | CG2 | VAL | D | 33 | 26.880 | 50.758 | 40.755 | 1.00 | 25.22 | C |
| ATOM | 2882 | N | PRO | D | 34 | 23.674 | 49.548 | 37.434 | 1.00 | 27.51 | N |
| ATOM | 2883 | CA | PRO | D | 34 | 23.085 | 49.608 | 36.105 | 1.00 | 28.26 | C |
| ATOM | 2884 | C | PRO | D | 34 | 23.491 | 50.909 | 35.413 | 1.00 | 31.20 | C |
| ATOM | 2885 | O | PRO | D | 34 | 23.649 | 51.980 | 36.012 | 1.00 | 32.62 | C |
| ATOM | 2886 | CB | PRO | D | 34 | 21.617 | 49.574 | 36.407 | 1.00 | 27.82 | C |
| ATOM | 2887 | CG | PRO | D | 34 | 21.523 | 48.866 | 37.750 | 1.00 | 29.77 | C |

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FIGURE 8A-59

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|-----|
| ATOM | 2888 | CD | PRO | D | 34 | 22.668 | 49.494 | 38.488 | 1.00 | 27.97 | C |
| ATOM | 2889 | N | GLY | D | 35 | 23.756 | 50.780 | 34.117 | 1.00 | 32.89 | N |
| ATOM | 2890 | CA | GLY | D | 35 | 24.265 | 51.891 | 33.338 | 1.00 | 34.68 | C |
| ATOM | 2891 | C | GLY | D | 35 | 25.749 | 52.065 | 33.438 | 1.00 | 34.91 | C |
| ATOM | 2892 | O | GLY | D | 35 | 26.271 | 53.066 | 32.991 | 1.00 | 38.32 | C |
| HETATM | 2893 | N | MSE | D | 36 | 26.456 | 51.105 | 33.995 | 1.00 | 36.03 | CON |
| HETATM | 2894 | CA | MSE | D | 36 | 27.910 | 51.084 | 34.060 | 1.00 | 38.11 | CON |
| HETATM | 2895 | C | MSE | D | 36 | 28.634 | 51.193 | 32.726 | 1.00 | 38.57 | CON |
| HETATM | 2896 | O | MSE | D | 36 | 29.741 | 51.717 | 32.594 | 1.00 | 39.99 | CO |
| HETATM | 2897 | CB | MSE | D | 36 | 28.255 | 49.744 | 34.622 | 1.00 | 41.60 | CC |
| HETATM | 2898 | CG | MSE | D | 36 | 28.972 | 49.795 | 35.911 | 1.00 | 45.00 | CC |
| HETATM | 2899 | SE | MSE | D | 36 | 30.412 | 48.532 | 35.745 | 1.00 | 54.90 | SE |
| HETATM | 2900 | CE | MSE | D | 36 | 30.966 | 48.492 | 33.897 | 1.00 | 45.21 | SE |
| ATOM | 2901 | N | ASP | D | 37 | 27.956 | 50.571 | 31.760 | 1.00 | 39.01 | NC |
| ATOM | 2902 | CA | ASP | D | 37 | 28.357 | 50.446 | 30.370 | 1.00 | 37.84 | CC |
| ATOM | 2903 | C | ASP | D | 37 | 28.125 | 51.687 | 29.525 | 1.00 | 37.29 | CO |
| ATOM | 2904 | O | ASP | D | 37 | 29.067 | 52.169 | 28.896 | 1.00 | 40.17 | CO |
| ATOM | 2905 | CB | ASP | D | 37 | 27.725 | 49.194 | 29.760 | 1.00 | 37.35 | CC |
| ATOM | 2906 | CG | ASP | D | 37 | 26.258 | 48.854 | 30.083 | 1.00 | 40.62 | CC |
| ATOM | 2907 | OD1 | ASP | D | 37 | 25.560 | 49.672 | 30.709 | 1.00 | 39.43 | CO |
| ATOM | 2908 | OD2 | ASP | D | 37 | 25.813 | 47.752 | 29.705 | 1.00 | 41.13 | CO |
| ATOM | 2909 | N | VAL | D | 38 | 26.930 | 52.266 | 29.525 | 1.00 | 36.85 | ON |
| ATOM | 2910 | CA | VAL | D | 38 | 26.665 | 53.462 | 28.719 | 1.00 | 38.43 | CC |
| ATOM | 2911 | C | VAL | D | 38 | 27.021 | 54.828 | 29.311 | 1.00 | 39.02 | CC |
| ATOM | 2912 | O | VAL | D | 38 | 27.395 | 55.748 | 28.581 | 1.00 | 39.83 | CO |
| ATOM | 2913 | CB | VAL | D | 38 | 25.212 | 53.466 | 28.171 | 1.00 | 36.76 | CC |
| ATOM | 2914 | CG1 | VAL | D | 38 | 25.086 | 52.227 | 27.356 | 1.00 | 36.24 | CC |
| ATOM | 2915 | CG2 | VAL | D | 38 | 24.081 | 53.482 | 29.175 | 1.00 | 36.31 | CC |
| ATOM | 2916 | N | LEU | D | 39 | 26.886 | 54.965 | 30.641 | 1.00 | 39.92 | CC |
| ATOM | 2917 | CA | LEU | D | 39 | 27.031 | 56.231 | 31.341 | 1.00 | 38.96 | CC |
| ATOM | 2918 | C | LEU | D | 39 | 28.495 | 56.624 | 31.625 | 1.00 | 41.40 | CC |
| ATOM | 2919 | O | LEU | D | 39 | 29.397 | 55.777 | 31.589 | 1.00 | 40.82 | CC |
| ATOM | 2920 | CB | LEU | D | 39 | 26.208 | 56.247 | 32.637 | 1.00 | 35.81 | CC |
| ATOM | 2921 | CG | LEU | D | 39 | 24.706 | 56.030 | 32.689 | 1.00 | 34.18 | CC |
| ATOM | 2922 | CD1 | LEU | D | 39 | 24.285 | 56.206 | 34.141 | 1.00 | 33.76 | CC |
| ATOM | 2923 | CD2 | LEU | D | 39 | 23.900 | 56.980 | 31.827 | 1.00 | 31.66 | CC |
| ATOM | 2924 | N | PRO | D | 40 | 28.807 | 57.926 | 31.852 | 1.00 | 44.17 | CC |
| ATOM | 2925 | CA | PRO | D | 40 | 30.141 | 58.383 | 32.244 | 1.00 | 44.44 | CC |
| ATOM | 2926 | C | PRO | D | 40 | 30.420 | 58.032 | 33.699 | 1.00 | 42.47 | CC |
| ATOM | 2927 | O | PRO | D | 40 | 29.550 | 58.003 | 34.562 | 1.00 | 42.05 | CC |
| ATOM | 2928 | CB | PRO | D | 40 | 30.115 | 59.908 | 32.011 | 1.00 | 45.14 | CC |
| ATOM | 2929 | CG | PRO | D | 40 | 28.674 | 60.256 | 32.263 | 1.00 | 45.10 | CC |
| ATOM | 2930 | CD | PRO | D | 40 | 27.934 | 59.092 | 31.603 | 1.00 | 46.22 | CC |
| ATOM | 2931 | N | SER | D | 41 | 31.694 | 57.749 | 33.906 | 1.00 | 42.00 | CC |
| ATOM | 2932 | CA | SER | D | 41 | 32.266 | 57.360 | 35.166 | 1.00 | 39.50 | CC |
| ATOM | 2933 | C | SER | D | 41 | 31.724 | 58.115 | 36.365 | 1.00 | 38.61 | CC |
| ATOM | 2934 | O | SER | D | 41 | 31.345 | 57.439 | 37.303 | 1.00 | 38.99 | CC |
| ATOM | 2935 | CB | SER | D | 41 | 33.760 | 57.491 | 35.009 | 1.00 | 40.43 | CC |
| ATOM | 2936 | OG | SER | D | 41 | 34.204 | 56.814 | 33.824 | 1.00 | 45.16 | CC |
| ATOM | 2937 | N | HIS | D | 42 | 31.550 | 59.442 | 36.396 | 1.00 | 38.17 | CC |
| ATOM | 2938 | CA | HIS | D | 42 | 31.018 | 60.127 | 37.567 | 1.00 | 36.99 | CC |
| ATOM | 2939 | C | HIS | D | 42 | 29.633 | 59.685 | 38.068 | 1.00 | 38.51 | CC |
| ATOM | 2940 | O | HIS | D | 42 | 29.219 | 59.978 | 39.190 | 1.00 | 39.73 | CC |
| ATOM | 2941 | CB | HIS | D | 42 | 31.062 | 61.646 | 37.328 | 1.00 | 36.53 | CC |
| ATOM | 2942 | CG | HIS | D | 42 | 29.988 | 62.146 | 36.370 | 1.00 | 34.40 | CC |
| ATOM | 2943 | ND1 | HIS | D | 42 | 30.070 | 62.275 | 35.063 | 1.00 | 35.82 | CC |
| ATOM | 2944 | CD2 | HIS | D | 42 | 28.694 | 62.443 | 36.749 | 1.00 | 36.22 | CC |
| ATOM | 2945 | CE1 | HIS | D | 42 | 28.872 | 62.607 | 34.629 | 1.00 | 35.92 | CC |
| ATOM | 2946 | NE2 | HIS | D | 42 | 28.050 | 62.680 | 35.644 | 1.00 | 37.56 | CC |
| ATOM | 2947 | N | CYS | D | 43 | 28.848 | 58.974 | 37.261 | 1.00 | 40.38 | N |

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FIGURE 8A-60

| | | | | | | | | | | | |
|--------|------|-----|-----|---|----|--------|--------|--------|------|-------|----|
| ATOM | 2948 | CA | CYS | D | 43 | 27.521 | 58.516 | 37.662 | 1.00 | 40.95 | C |
| ATOM | 2949 | C | CYS | D | 43 | 27.545 | 57.165 | 38.394 | 1.00 | 38.66 | C |
| ATOM | 2950 | O | CYS | D | 43 | 26.556 | 56.769 | 39.027 | 1.00 | 38.58 | O |
| ATOM | 2951 | CB | CYS | D | 43 | 26.561 | 58.489 | 36.426 | 1.00 | 43.16 | C |
| ATOM | 2952 | SG | CYS | D | 43 | 25.889 | 60.126 | 35.971 | 1.00 | 50.07 | O |
| ATOM | 2953 | N | TRP | D | 44 | 28.677 | 56.450 | 38.300 | 1.00 | 34.96 | N |
| ATOM | 2954 | CA | TRP | D | 44 | 28.763 | 55.094 | 38.789 | 1.00 | 32.27 | C |
| ATOM | 2955 | C | TRP | D | 44 | 30.055 | 54.754 | 39.486 | 1.00 | 32.35 | C |
| ATOM | 2956 | O | TRP | D | 44 | 30.010 | 53.891 | 40.349 | 1.00 | 34.30 | O |
| ATOM | 2957 | CB | TRP | D | 44 | 28.502 | 54.045 | 37.688 | 1.00 | 29.74 | C |
| ATOM | 2958 | CG | TRP | D | 44 | 29.428 | 54.039 | 36.479 | 1.00 | 25.62 | C |
| ATOM | 2959 | CD1 | TRP | D | 44 | 29.034 | 54.689 | 35.340 | 1.00 | 24.56 | C |
| ATOM | 2960 | CD2 | TRP | D | 44 | 30.636 | 53.392 | 36.360 | 1.00 | 24.29 | C |
| ATOM | 2961 | NE1 | TRP | D | 44 | 30.006 | 54.462 | 34.497 | 1.00 | 26.57 | N |
| ATOM | 2962 | CE2 | TRP | D | 44 | 30.972 | 53.705 | 35.046 | 1.00 | 25.16 | C |
| ATOM | 2963 | CE3 | TRP | D | 44 | 31.442 | 52.536 | 37.072 | 1.00 | 21.05 | C |
| ATOM | 2964 | CZ2 | TRP | D | 44 | 32.119 | 53.210 | 34.446 | 1.00 | 23.57 | C |
| ATOM | 2965 | CZ3 | TRP | D | 44 | 32.600 | 52.058 | 36.490 | 1.00 | 21.72 | C |
| ATOM | 2966 | CH2 | TRP | D | 44 | 32.956 | 52.395 | 35.194 | 1.00 | 23.72 | C |
| ATOM | 2967 | N | ILE | D | 45 | 31.191 | 55.378 | 39.216 | 1.00 | 31.34 | N |
| ATOM | 2968 | CA | ILE | D | 45 | 32.444 | 54.851 | 39.687 | 1.00 | 34.23 | C |
| ATOM | 2969 | C | ILE | D | 45 | 32.627 | 54.719 | 41.206 | 1.00 | 35.04 | C |
| ATOM | 2970 | O | ILE | D | 45 | 33.222 | 53.726 | 41.618 | 1.00 | 36.05 | O |
| ATOM | 2971 | CB | ILE | D | 45 | 33.586 | 55.584 | 38.980 | 1.00 | 35.62 | C |
| ATOM | 2972 | CG1 | ILE | D | 45 | 34.959 | 54.917 | 39.068 | 1.00 | 36.05 | C |
| ATOM | 2973 | CG2 | ILE | D | 45 | 33.716 | 56.959 | 39.592 | 1.00 | 37.86 | C |
| ATOM | 2974 | CD1 | ILE | D | 45 | 35.020 | 53.482 | 38.545 | 1.00 | 36.81 | C |
| ATOM | 2975 | N | SER | D | 46 | 32.100 | 55.591 | 42.080 | 1.00 | 35.07 | N |
| ATOM | 2976 | CA | SER | D | 46 | 32.421 | 55.538 | 43.500 | 1.00 | 35.85 | C |
| ATOM | 2977 | C | SER | D | 46 | 31.651 | 54.443 | 44.213 | 1.00 | 35.51 | C |
| ATOM | 2978 | O | SER | D | 46 | 32.169 | 53.858 | 45.165 | 1.00 | 38.41 | O |
| ATOM | 2979 | CB | SER | D | 46 | 32.165 | 56.852 | 44.223 | 1.00 | 36.96 | C |
| ATOM | 2980 | OG | SER | D | 46 | 30.786 | 57.005 | 44.534 | 1.00 | 40.12 | O |
| ATOM | 2981 | N | GLU | D | 47 | 30.419 | 54.185 | 43.770 | 1.00 | 33.93 | N |
| ATOM | 2982 | CA | GLU | D | 47 | 29.656 | 53.051 | 44.230 | 1.00 | 32.65 | C |
| ATOM | 2983 | C | GLU | D | 47 | 30.197 | 51.773 | 43.648 | 1.00 | 31.56 | C |
| ATOM | 2984 | O | GLU | D | 47 | 30.216 | 50.761 | 44.339 | 1.00 | 31.25 | O |
| ATOM | 2985 | CB | GLU | D | 47 | 28.206 | 53.193 | 43.842 | 1.00 | 36.42 | C |
| ATOM | 2986 | CG | GLU | D | 47 | 27.306 | 51.989 | 44.164 | 1.00 | 45.32 | C |
| ATOM | 2987 | CD | GLU | D | 47 | 26.964 | 51.716 | 45.628 | 1.00 | 48.90 | C |
| ATOM | 2988 | OE1 | GLU | D | 47 | 27.839 | 51.323 | 46.399 | 1.00 | 52.24 | O |
| ATOM | 2989 | OE2 | GLU | D | 47 | 25.797 | 51.872 | 45.995 | 1.00 | 52.95 | O |
| HETATM | 2990 | N | MSE | D | 48 | 30.646 | 51.788 | 42.398 | 1.00 | 30.45 | N |
| HETATM | 2991 | CA | MSE | D | 48 | 31.189 | 50.592 | 41.798 | 1.00 | 31.67 | C |
| HETATM | 2992 | C | MSE | D | 48 | 32.499 | 50.155 | 42.444 | 1.00 | 30.88 | C |
| HETATM | 2993 | O | MSE | D | 48 | 32.694 | 48.961 | 42.577 | 1.00 | 33.46 | O |
| HETATM | 2994 | CB | MSE | D | 48 | 31.394 | 50.777 | 40.342 | 1.00 | 32.74 | C |
| HETATM | 2995 | CG | MSE | D | 48 | 31.510 | 49.459 | 39.632 | 1.00 | 36.29 | C |
| HETATM | 2996 | SE | MSE | D | 48 | 29.910 | 48.366 | 39.787 | 1.00 | 47.34 | SE |
| HETATM | 2997 | CE | MSE | D | 48 | 30.895 | 46.927 | 39.264 | 1.00 | 38.75 | C |
| ATOM | 2998 | N | VAL | D | 49 | 33.433 | 50.984 | 42.904 | 1.00 | 30.60 | N |
| ATOM | 2999 | CA | VAL | D | 49 | 34.605 | 50.504 | 43.671 | 1.00 | 29.47 | C |
| ATOM | 3000 | C | VAL | D | 49 | 34.285 | 50.012 | 45.074 | 1.00 | 27.89 | C |
| ATOM | 3001 | O | VAL | D | 49 | 34.967 | 49.128 | 45.596 | 1.00 | 27.63 | O |
| ATOM | 3002 | CB | VAL | D | 49 | 35.828 | 51.488 | 43.781 | 1.00 | 30.38 | C |
| ATOM | 3003 | CG1 | VAL | D | 49 | 36.552 | 51.617 | 42.439 | 1.00 | 30.57 | C |
| ATOM | 3004 | CG2 | VAL | D | 49 | 35.440 | 52.863 | 44.340 | 1.00 | 30.43 | C |
| ATOM | 3005 | N | VAL | D | 50 | 33.263 | 50.622 | 45.679 | 1.00 | 25.21 | N |
| ATOM | 3006 | CA | VAL | D | 50 | 32.754 | 50.149 | 46.945 | 1.00 | 24.70 | C |
| ATOM | 3007 | C | VAL | D | 50 | 32.153 | 48.745 | 46.832 | 1.00 | 24.08 | C |

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FIGURE 8A-61

| | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 3008 | O | VAL | D | 50 | 32.438 | 47.921 | 47.699 | 1.00 | 25.08 |
| ATOM | 3009 | CB | VAL | D | 50 | 31.757 | 51.172 | 47.504 | 1.00 | 24.15 |
| ATOM | 3010 | CG1 | VAL | D | 50 | 30.945 | 50.583 | 48.650 | 1.00 | 24.85 |
| ATOM | 3011 | CG2 | VAL | D | 50 | 32.484 | 52.411 | 47.974 | 1.00 | 21.01 |
| ATOM | 3012 | N | GLN | D | 51 | 31.343 | 48.470 | 45.796 | 1.00 | 22.06 |
| ATOM | 3013 | CA | GLN | D | 51 | 30.807 | 47.154 | 45.522 | 1.00 | 22.13 |
| ATOM | 3014 | C | GLN | D | 51 | 31.810 | 46.099 | 45.123 | 1.00 | 20.89 |
| ATOM | 3015 | O | GLN | D | 51 | 31.663 | 44.940 | 45.479 | 1.00 | 21.33 |
| ATOM | 3016 | CB | GLN | D | 51 | 29.719 | 47.249 | 44.484 | 1.00 | 24.57 |
| ATOM | 3017 | CG | GLN | D | 51 | 28.496 | 47.999 | 45.018 | 1.00 | 26.12 |
| ATOM | 3018 | CD | GLN | D | 51 | 27.936 | 47.379 | 46.304 | 1.00 | 26.75 |
| ATOM | 3019 | OE1 | GLN | D | 51 | 28.128 | 46.194 | 46.616 | 1.00 | 25.54 |
| ATOM | 3020 | NE2 | GLN | D | 51 | 27.234 | 48.198 | 47.088 | 1.00 | 26.23 |
| ATOM | 3021 | N | LEU | D | 52 | 32.839 | 46.544 | 44.423 | 1.00 | 19.69 |
| ATOM | 3022 | CA | LEU | D | 52 | 33.966 | 45.728 | 44.057 | 1.00 | 20.34 |
| ATOM | 3023 | C | LEU | D | 52 | 34.831 | 45.383 | 45.250 | 1.00 | 20.47 |
| ATOM | 3024 | O | LEU | D | 52 | 35.199 | 44.215 | 45.356 | 1.00 | 23.75 |
| ATOM | 3025 | CB | LEU | D | 52 | 34.866 | 46.398 | 42.976 | 1.00 | 19.72 |
| ATOM | 3026 | CG | LEU | D | 52 | 34.402 | 46.541 | 41.509 | 1.00 | 18.02 |
| ATOM | 3027 | CD1 | LEU | D | 52 | 35.404 | 47.412 | 40.807 | 1.00 | 14.47 |
| ATOM | 3028 | CD2 | LEU | D | 52 | 34.217 | 45.177 | 40.844 | 1.00 | 14.93 |
| ATOM | 3029 | N | SER | D | 53 | 35.178 | 46.294 | 46.165 | 1.00 | 21.36 |
| ATOM | 3030 | CA | SER | D | 53 | 35.913 | 45.942 | 47.377 | 1.00 | 22.45 |
| ATOM | 3031 | C | SER | D | 53 | 35.173 | 44.873 | 48.166 | 1.00 | 22.70 |
| ATOM | 3032 | O | SER | D | 53 | 35.770 | 43.895 | 48.565 | 1.00 | 24.55 |
| ATOM | 3033 | CB | SER | D | 53 | 36.117 | 47.178 | 48.233 | 1.00 | 25.43 |
| ATOM | 3034 | OG | SER | D | 53 | 36.882 | 46.917 | 49.410 | 1.00 | 32.17 |
| ATOM | 3035 | N | ASP | D | 54 | 33.852 | 44.962 | 48.286 | 1.00 | 23.74 |
| ATOM | 3036 | CA | ASP | D | 54 | 33.021 | 44.038 | 49.030 | 1.00 | 25.51 |
| ATOM | 3037 | C | ASP | D | 54 | 33.119 | 42.633 | 48.500 | 1.00 | 22.56 |
| ATOM | 3038 | O | ASP | D | 54 | 33.390 | 41.711 | 49.250 | 1.00 | 22.33 |
| ATOM | 3039 | CB | ASP | D | 54 | 31.565 | 44.500 | 48.963 | 1.00 | 32.00 |
| ATOM | 3040 | CG | ASP | D | 54 | 30.624 | 43.913 | 50.019 | 1.00 | 42.23 |
| ATOM | 3041 | OD1 | ASP | D | 54 | 30.117 | 42.792 | 49.841 | 1.00 | 45.21 |
| ATOM | 3042 | OD2 | ASP | D | 54 | 30.364 | 44.607 | 51.018 | 1.00 | 49.94 |
| ATOM | 3043 | N | SER | D | 55 | 32.943 | 42.520 | 47.192 | 1.00 | 19.99 |
| ATOM | 3044 | CA | SER | D | 55 | 32.933 | 41.258 | 46.504 | 1.00 | 16.42 |
| ATOM | 3045 | C | SER | D | 55 | 34.279 | 40.596 | 46.521 | 1.00 | 14.71 |
| ATOM | 3046 | O | SER | D | 55 | 34.395 | 39.393 | 46.693 | 1.00 | 15.83 |
| ATOM | 3047 | CB | SER | D | 55 | 32.503 | 41.468 | 45.066 | 1.00 | 16.29 |
| ATOM | 3048 | OG | SER | D | 55 | 31.170 | 41.909 | 44.886 | 1.00 | 19.97 |
| ATOM | 3049 | N | LEU | D | 56 | 35.296 | 41.406 | 46.315 | 1.00 | 15.85 |
| ATOM | 3050 | CA | LEU | D | 56 | 36.638 | 40.884 | 46.345 | 1.00 | 17.57 |
| ATOM | 3051 | C | LEU | D | 56 | 37.034 | 40.485 | 47.744 | 1.00 | 17.75 |
| ATOM | 3052 | O | LEU | D | 56 | 37.782 | 39.527 | 47.863 | 1.00 | 19.01 |
| ATOM | 3053 | CB | LEU | D | 56 | 37.619 | 41.904 | 45.848 | 1.00 | 17.61 |
| ATOM | 3054 | CG | LEU | D | 56 | 37.813 | 42.091 | 44.344 | 1.00 | 21.27 |
| ATOM | 3055 | CD1 | LEU | D | 56 | 38.577 | 43.396 | 44.141 | 1.00 | 19.96 |
| ATOM | 3056 | CD2 | LEU | D | 56 | 38.540 | 40.936 | 43.687 | 1.00 | 16.32 |
| ATOM | 3057 | N | THR | D | 57 | 36.560 | 41.169 | 48.803 | 1.00 | 19.07 |
| ATOM | 3058 | CA | THR | D | 57 | 36.864 | 40.818 | 50.189 | 1.00 | 17.97 |
| ATOM | 3059 | C | THR | D | 57 | 36.126 | 39.571 | 50.566 | 1.00 | 18.20 |
| ATOM | 3060 | O | THR | D | 57 | 36.674 | 38.746 | 51.266 | 1.00 | 20.89 |
| ATOM | 3061 | CB | THR | D | 57 | 36.521 | 41.984 | 51.099 | 1.00 | 19.37 |
| ATOM | 3062 | OG1 | THR | D | 57 | 37.503 | 42.932 | 50.741 | 1.00 | 20.91 |
| ATOM | 3063 | CG2 | THR | D | 57 | 36.778 | 41.786 | 52.575 | 1.00 | 26.13 |
| ATOM | 3064 | N | ASP | D | 58 | 34.924 | 39.346 | 50.085 | 1.00 | 18.03 |
| ATOM | 3065 | CA | ASP | D | 58 | 34.293 | 38.066 | 50.220 | 1.00 | 18.76 |
| ATOM | 3066 | C | ASP | D | 58 | 34.958 | 37.009 | 49.397 | 1.00 | 20.46 |
| ATOM | 3067 | O | ASP | D | 58 | 35.041 | 35.878 | 49.865 | 1.00 | 20.47 |

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FIGURE 8A-62

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 3068 | CB | ASP | D | 58 | 32.859 | 38.102 | 49.791 | 1.00 | 21.24 | C |
| ATOM | 3069 | CG | ASP | D | 58 | 32.043 | 39.157 | 50.517 | 1.00 | 26.19 | C |
| ATOM | 3070 | OD1 | ASP | D | 58 | 32.458 | 39.665 | 51.572 | 1.00 | 26.83 | O |
| ATOM | 3071 | OD2 | ASP | D | 58 | 30.970 | 39.481 | 49.993 | 1.00 | 30.50 | O |
| ATOM | 3072 | N | LEU | D | 59 | 35.449 | 37.324 | 48.197 | 1.00 | 19.65 | N |
| ATOM | 3073 | CA | LEU | D | 59 | 36.099 | 36.331 | 47.383 | 1.00 | 18.09 | C |
| ATOM | 3074 | C | LEU | D | 59 | 37.345 | 35.878 | 48.090 | 1.00 | 19.12 | C |
| ATOM | 3075 | O | LEU | D | 59 | 37.553 | 34.694 | 48.251 | 1.00 | 23.04 | C |
| ATOM | 3076 | CB | LEU | D | 59 | 36.392 | 36.893 | 46.028 | 1.00 | 16.75 | O |
| ATOM | 3077 | CG | LEU | D | 59 | 36.808 | 35.864 | 45.048 | 1.00 | 17.14 | C |
| ATOM | 3078 | CD1 | LEU | D | 59 | 35.714 | 34.823 | 44.909 | 1.00 | 16.41 | C |
| ATOM | 3079 | CD2 | LEU | D | 59 | 37.209 | 36.546 | 43.769 | 1.00 | 16.93 | C |
| ATOM | 3080 | N | LEU | D | 60 | 38.132 | 36.764 | 48.667 | 1.00 | 21.47 | N |
| ATOM | 3081 | CA | LEU | D | 60 | 39.332 | 36.428 | 49.431 | 1.00 | 22.73 | C |
| ATOM | 3082 | C | LEU | D | 60 | 39.173 | 35.401 | 50.564 | 1.00 | 24.38 | C |
| ATOM | 3083 | O | LEU | D | 60 | 40.084 | 34.626 | 50.853 | 1.00 | 25.12 | O |
| ATOM | 3084 | CB | LEU | D | 60 | 39.852 | 37.726 | 50.017 | 1.00 | 21.70 | C |
| ATOM | 3085 | CG | LEU | D | 60 | 41.196 | 37.710 | 50.670 | 1.00 | 23.77 | C |
| ATOM | 3086 | CD1 | LEU | D | 60 | 42.256 | 37.514 | 49.598 | 1.00 | 22.63 | C |
| ATOM | 3087 | CD2 | LEU | D | 60 | 41.446 | 38.985 | 51.425 | 1.00 | 24.99 | C |
| ATOM | 3088 | N | ASP | D | 61 | 38.005 | 35.386 | 51.224 | 1.00 | 26.63 | N |
| ATOM | 3089 | CA | ASP | D | 61 | 37.705 | 34.524 | 52.363 | 1.00 | 25.59 | C |
| ATOM | 3090 | C | ASP | D | 61 | 37.428 | 33.112 | 51.872 | 1.00 | 22.43 | C |
| ATOM | 3091 | O | ASP | D | 61 | 37.373 | 32.161 | 52.646 | 1.00 | 23.39 | O |
| ATOM | 3092 | CB | ASP | D | 61 | 36.497 | 35.146 | 53.120 | 1.00 | 33.33 | C |
| ATOM | 3093 | CG | ASP | D | 61 | 35.889 | 34.390 | 54.325 | 1.00 | 40.36 | C |
| ATOM | 3094 | OD1 | ASP | D | 61 | 36.478 | 34.403 | 55.424 | 1.00 | 44.78 | O |
| ATOM | 3095 | OD2 | ASP | D | 61 | 34.807 | 33.794 | 54.169 | 1.00 | 43.10 | O |
| ATOM | 3096 | N | LYS | D | 62 | 37.289 | 32.899 | 50.575 | 1.00 | 17.94 | N |
| ATOM | 3097 | CA | LYS | D | 62 | 37.048 | 31.574 | 50.058 | 1.00 | 13.29 | C |
| ATOM | 3098 | C | LYS | D | 62 | 38.344 | 30.855 | 49.757 | 1.00 | 12.68 | C |
| ATOM | 3099 | O | LYS | D | 62 | 38.308 | 29.692 | 49.387 | 1.00 | 15.69 | O |
| ATOM | 3100 | CB | LYS | D | 62 | 36.292 | 31.712 | 48.771 | 1.00 | 13.99 | C |
| ATOM | 3101 | CG | LYS | D | 62 | 35.036 | 32.517 | 48.890 | 1.00 | 16.25 | C |
| ATOM | 3102 | CD | LYS | D | 62 | 34.086 | 31.871 | 49.870 | 1.00 | 21.21 | C |
| ATOM | 3103 | CE | LYS | D | 62 | 32.997 | 32.898 | 50.166 | 1.00 | 23.50 | C |
| ATOM | 3104 | NZ | LYS | D | 62 | 32.319 | 33.267 | 48.937 | 1.00 | 30.45 | N |
| ATOM | 3105 | N | PHE | D | 63 | 39.504 | 31.504 | 49.885 | 1.00 | 12.18 | N |
| ATOM | 3106 | CA | PHE | D | 63 | 40.797 | 30.938 | 49.594 | 1.00 | 13.29 | C |
| ATOM | 3107 | C | PHE | D | 63 | 41.659 | 30.965 | 50.837 | 1.00 | 16.38 | C |
| ATOM | 3108 | O | PHE | D | 63 | 41.401 | 31.701 | 51.798 | 1.00 | 16.40 | O |
| ATOM | 3109 | CB | PHE | D | 63 | 41.495 | 31.773 | 48.552 | 1.00 | 11.01 | C |
| ATOM | 3110 | CG | PHE | D | 63 | 40.776 | 31.641 | 47.229 | 1.00 | 13.33 | C |
| ATOM | 3111 | CD1 | PHE | D | 63 | 40.917 | 30.478 | 46.491 | 1.00 | 11.26 | C |
| ATOM | 3112 | CD2 | PHE | D | 63 | 39.904 | 32.635 | 46.823 | 1.00 | 13.18 | C |
| ATOM | 3113 | CE1 | PHE | D | 63 | 40.140 | 30.299 | 45.367 | 1.00 | 9.84 | C |
| ATOM | 3114 | CE2 | PHE | D | 63 | 39.126 | 32.436 | 45.690 | 1.00 | 13.90 | C |
| ATOM | 3115 | CZ | PHE | D | 63 | 39.251 | 31.264 | 44.964 | 1.00 | 10.53 | C |
| ATOM | 3116 | N | SER | D | 64 | 42.725 | 30.164 | 50.773 | 1.00 | 16.82 | N |
| ATOM | 3117 | CA | SER | D | 64 | 43.703 | 30.208 | 51.822 | 1.00 | 16.74 | C |
| ATOM | 3118 | C | SER | D | 64 | 45.123 | 30.230 | 51.275 | 1.00 | 16.89 | C |
| ATOM | 3119 | O | SER | D | 64 | 45.377 | 29.918 | 50.120 | 1.00 | 16.97 | O |
| ATOM | 3120 | CB | SER | D | 64 | 43.430 | 29.068 | 52.849 | 1.00 | 18.93 | C |
| ATOM | 3121 | OG | SER | D | 64 | 44.080 | 27.847 | 52.508 | 1.00 | 28.24 | O |
| ATOM | 3122 | N | ASN | D | 65 | 46.080 | 30.661 | 52.095 | 1.00 | 16.96 | N |
| ATOM | 3123 | CA | ASN | D | 65 | 47.479 | 30.684 | 51.746 | 1.00 | 15.98 | C |
| ATOM | 3124 | C | ASN | D | 65 | 48.027 | 29.319 | 51.496 | 1.00 | 15.15 | C |
| ATOM | 3125 | O | ASN | D | 65 | 47.472 | 28.362 | 52.000 | 1.00 | 17.07 | O |
| ATOM | 3126 | CB | ASN | D | 65 | 48.341 | 31.398 | 52.774 | 1.00 | 17.48 | C |
| ATOM | 3127 | CG | ASN | D | 65 | 48.232 | 32.904 | 52.684 | 1.00 | 19.71 | C |

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FIGURE 8A-63

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 3128 | OD1 | ASN | D | 65 | 48.695 | 33.551 | 51.752 | 1.00 | 25.73 | O |
| ATOM | 3129 | ND2 | ASN | D | 65 | 47.621 | 33.560 | 53.640 | 1.00 | 22.21 | N |
| ATOM | 3130 | N | ILE | D | 66 | 49.077 | 29.253 | 50.672 | 1.00 | 15.61 | C |
| ATOM | 3131 | CA | ILE | D | 66 | 49.778 | 28.029 | 50.363 | 1.00 | 16.53 | C |
| ATOM | 3132 | C | ILE | D | 66 | 51.232 | 28.235 | 50.711 | 1.00 | 16.49 | O |
| ATOM | 3133 | O | ILE | D | 66 | 51.633 | 29.383 | 50.813 | 1.00 | 17.79 | C |
| ATOM | 3134 | CB | ILE | D | 66 | 49.594 | 27.623 | 48.869 | 1.00 | 16.19 | C |
| ATOM | 3135 | CG1 | ILE | D | 66 | 50.149 | 28.660 | 47.906 | 1.00 | 16.66 | C |
| ATOM | 3136 | CG2 | ILE | D | 66 | 48.115 | 27.329 | 48.611 | 1.00 | 12.63 | C |
| ATOM | 3137 | CD1 | ILE | D | 66 | 50.081 | 28.086 | 46.478 | 1.00 | 18.10 | C |
| ATOM | 3138 | N | SER | D | 67 | 52.041 | 27.187 | 50.853 | 1.00 | 18.84 | N |
| ATOM | 3139 | CA | SER | D | 67 | 53.442 | 27.347 | 51.233 | 1.00 | 23.17 | C |
| ATOM | 3140 | C | SER | D | 67 | 54.305 | 28.078 | 50.214 | 1.00 | 23.34 | C |
| ATOM | 3141 | O | SER | D | 67 | 55.250 | 28.779 | 50.552 | 1.00 | 25.92 | O |
| ATOM | 3142 | CB | SER | D | 67 | 54.084 | 26.006 | 51.543 | 1.00 | 23.00 | O |
| ATOM | 3143 | OG | SER | D | 67 | 53.971 | 25.139 | 50.419 | 1.00 | 30.06 | O |
| ATOM | 3144 | N | GLU | D | 68 | 53.981 | 27.968 | 48.942 | 1.00 | 25.32 | N |
| ATOM | 3145 | CA | GLU | D | 68 | 54.755 | 28.626 | 47.914 | 1.00 | 27.08 | C |
| ATOM | 3146 | C | GLU | D | 68 | 54.045 | 28.401 | 46.597 | 1.00 | 25.08 | C |
| ATOM | 3147 | O | GLU | D | 68 | 53.391 | 27.373 | 46.403 | 1.00 | 24.26 | O |
| ATOM | 3148 | CB | GLU | D | 68 | 56.190 | 28.061 | 47.921 | 1.00 | 30.32 | O |
| ATOM | 3149 | CG | GLU | D | 68 | 56.711 | 27.081 | 46.883 | 1.00 | 40.98 | C |
| ATOM | 3150 | CD | GLU | D | 68 | 56.009 | 25.744 | 46.778 | 1.00 | 46.80 | C |
| ATOM | 3151 | OE1 | GLU | D | 68 | 55.947 | 24.998 | 47.773 | 1.00 | 50.12 | O |
| ATOM | 3152 | OE2 | GLU | D | 68 | 55.508 | 25.470 | 45.676 | 1.00 | 52.68 | O |
| ATOM | 3153 | N | GLY | D | 69 | 54.121 | 29.389 | 45.723 | 1.00 | 23.65 | N |
| ATOM | 3154 | CA | GLY | D | 69 | 53.784 | 29.192 | 44.320 | 1.00 | 24.95 | C |
| ATOM | 3155 | C | GLY | D | 69 | 52.580 | 30.012 | 43.952 | 1.00 | 23.05 | C |
| ATOM | 3156 | O | GLY | D | 69 | 52.270 | 30.941 | 44.691 | 1.00 | 24.04 | O |
| ATOM | 3157 | N | LEU | D | 70 | 51.883 | 29.667 | 42.870 | 1.00 | 22.75 | N |
| ATOM | 3158 | CA | LEU | D | 70 | 50.768 | 30.474 | 42.415 | 1.00 | 23.31 | C |
| ATOM | 3159 | C | LEU | D | 70 | 49.618 | 30.380 | 43.412 | 1.00 | 21.85 | C |
| ATOM | 3160 | O | LEU | D | 70 | 49.170 | 29.262 | 43.689 | 1.00 | 23.27 | O |
| ATOM | 3161 | CB | LEU | D | 70 | 50.307 | 29.902 | 41.114 | 1.00 | 22.88 | O |
| ATOM | 3162 | CG | LEU | D | 70 | 49.652 | 30.850 | 40.145 | 1.00 | 22.31 | C |
| ATOM | 3163 | CD1 | LEU | D | 70 | 49.073 | 29.925 | 39.088 | 1.00 | 24.98 | C |
| ATOM | 3164 | CD2 | LEU | D | 70 | 48.576 | 31.722 | 40.710 | 1.00 | 21.90 | C |
| ATOM | 3165 | N | SER | D | 71 | 49.143 | 31.526 | 43.918 | 1.00 | 19.05 | C |
| ATOM | 3166 | CA | SER | D | 71 | 48.132 | 31.561 | 44.977 | 1.00 | 16.36 | C |
| ATOM | 3167 | C | SER | D | 71 | 47.008 | 32.518 | 44.667 | 1.00 | 15.90 | C |
| ATOM | 3168 | O | SER | D | 71 | 47.262 | 33.701 | 44.521 | 1.00 | 18.19 | O |
| ATOM | 3169 | CB | SER | D | 71 | 48.747 | 32.015 | 46.298 | 1.00 | 15.26 | C |
| ATOM | 3170 | OG | SER | D | 71 | 47.822 | 32.217 | 47.360 | 1.00 | 16.34 | O |
| ATOM | 3171 | N | ASN | D | 72 | 45.757 | 32.053 | 44.598 | 1.00 | 17.24 | N |
| ATOM | 3172 | CA | ASN | D | 72 | 44.604 | 32.871 | 44.335 | 1.00 | 14.30 | C |
| ATOM | 3173 | C | ASN | D | 72 | 44.451 | 33.836 | 45.493 | 1.00 | 16.33 | C |
| ATOM | 3174 | O | ASN | D | 72 | 44.170 | 35.023 | 45.286 | 1.00 | 16.94 | O |
| ATOM | 3175 | CB | ASN | D | 72 | 43.399 | 31.967 | 44.208 | 1.00 | 14.51 | C |
| ATOM | 3176 | CG | ASN | D | 72 | 43.311 | 31.102 | 42.953 | 1.00 | 14.36 | C |
| ATOM | 3177 | OD1 | ASN | D | 72 | 44.170 | 31.156 | 42.089 | 1.00 | 15.41 | O |
| ATOM | 3178 | ND2 | ASN | D | 72 | 42.291 | 30.261 | 42.779 | 1.00 | 14.10 | N |
| ATOM | 3179 | N | TYR | D | 73 | 44.711 | 33.348 | 46.720 | 1.00 | 16.70 | N |
| ATOM | 3180 | CA | TYR | D | 73 | 44.709 | 34.222 | 47.893 | 1.00 | 17.86 | C |
| ATOM | 3181 | C | TYR | D | 73 | 45.580 | 35.466 | 47.698 | 1.00 | 17.22 | C |
| ATOM | 3182 | O | TYR | D | 73 | 45.047 | 36.559 | 47.813 | 1.00 | 19.51 | O |
| ATOM | 3183 | CB | TYR | D | 73 | 45.171 | 33.479 | 49.182 | 1.00 | 15.83 | C |
| ATOM | 3184 | CG | TYR | D | 73 | 44.962 | 34.331 | 50.421 | 1.00 | 11.11 | C |
| ATOM | 3185 | CD1 | TYR | D | 73 | 43.755 | 34.297 | 51.064 | 1.00 | 13.95 | C |
| ATOM | 3186 | CD2 | TYR | D | 73 | 45.932 | 35.212 | 50.823 | 1.00 | 14.63 | C |
| ATOM | 3187 | CE1 | TYR | D | 73 | 43.474 | 35.184 | 52.080 | 1.00 | 15.34 | C |

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FIGURE 8A-64

| | | | | | | | | | | | |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 3188 | CE2 | TYR | D | 73 | 45.663 | 36.140 | 51.814 | 1.00 | 15.34 | C |
| ATOM | 3189 | CZ | TYR | D | 73 | 44.430 | 36.108 | 52.407 | 1.00 | 16.30 | C |
| ATOM | 3190 | OH | TYR | D | 73 | 44.123 | 37.051 | 53.334 | 1.00 | 22.01 | C |
| ATOM | 3191 | N | SER | D | 74 | 46.888 | 35.357 | 47.402 | 1.00 | 18.57 | N |
| ATOM | 3192 | CA | SER | D | 74 | 47.786 | 36.498 | 47.221 | 1.00 | 17.90 | C |
| ATOM | 3193 | C | SER | D | 74 | 47.420 | 37.417 | 46.121 | 1.00 | 16.44 | C |
| ATOM | 3194 | O | SER | D | 74 | 47.636 | 38.600 | 46.291 | 1.00 | 18.01 | C |
| ATOM | 3195 | CB | SER | D | 74 | 49.180 | 36.125 | 46.829 | 1.00 | 18.93 | O |
| ATOM | 3196 | OG | SER | D | 74 | 49.623 | 35.176 | 47.760 | 1.00 | 25.77 | C |
| ATOM | 3197 | N | ILE | D | 75 | 46.890 | 36.866 | 45.027 | 1.00 | 16.68 | N |
| ATOM | 3198 | CA | ILE | D | 75 | 46.470 | 37.645 | 43.893 | 1.00 | 16.88 | C |
| ATOM | 3199 | C | ILE | D | 75 | 45.256 | 38.493 | 44.244 | 1.00 | 16.78 | C |
| ATOM | 3200 | O | ILE | D | 75 | 45.237 | 39.693 | 43.968 | 1.00 | 20.42 | C |
| ATOM | 3201 | CB | ILE | D | 75 | 46.184 | 36.709 | 42.711 | 1.00 | 16.41 | O |
| ATOM | 3202 | CG1 | ILE | D | 75 | 47.380 | 35.898 | 42.295 | 1.00 | 16.78 | C |
| ATOM | 3203 | CG2 | ILE | D | 75 | 45.861 | 37.615 | 41.567 | 1.00 | 16.46 | C |
| ATOM | 3204 | CD1 | ILE | D | 75 | 47.146 | 34.967 | 41.097 | 1.00 | 19.66 | C |
| ATOM | 3205 | N | ILE | D | 76 | 44.230 | 37.936 | 44.901 | 1.00 | 18.21 | N |
| ATOM | 3206 | CA | ILE | D | 76 | 43.023 | 38.678 | 45.220 | 1.00 | 15.41 | C |
| ATOM | 3207 | C | ILE | D | 76 | 43.340 | 39.669 | 46.286 | 1.00 | 17.60 | C |
| ATOM | 3208 | O | ILE | D | 76 | 42.870 | 40.796 | 46.215 | 1.00 | 20.17 | C |
| ATOM | 3209 | CB | ILE | D | 76 | 41.941 | 37.743 | 45.711 | 1.00 | 16.42 | O |
| ATOM | 3210 | CG1 | ILE | D | 76 | 41.615 | 36.789 | 44.588 | 1.00 | 14.92 | C |
| ATOM | 3211 | CG2 | ILE | D | 76 | 40.696 | 38.481 | 46.200 | 1.00 | 11.21 | C |
| ATOM | 3212 | CD1 | ILE | D | 76 | 40.745 | 35.613 | 45.055 | 1.00 | 13.69 | C |
| ATOM | 3213 | N | ASP | D | 77 | 44.162 | 39.271 | 47.248 | 1.00 | 19.35 | N |
| ATOM | 3214 | CA | ASP | D | 77 | 44.561 | 40.150 | 48.321 | 1.00 | 21.77 | C |
| ATOM | 3215 | C | ASP | D | 77 | 45.248 | 41.436 | 47.858 | 1.00 | 22.56 | C |
| ATOM | 3216 | O | ASP | D | 77 | 44.924 | 42.515 | 48.376 | 1.00 | 22.07 | O |
| ATOM | 3217 | CB | ASP | D | 77 | 45.433 | 39.385 | 49.282 | 1.00 | 24.17 | C |
| ATOM | 3218 | CG | ASP | D | 77 | 45.713 | 40.148 | 50.571 | 1.00 | 28.55 | C |
| ATOM | 3219 | OD1 | ASP | D | 77 | 44.842 | 40.889 | 51.067 | 1.00 | 33.63 | O |
| ATOM | 3220 | OD2 | ASP | D | 77 | 46.822 | 39.988 | 51.073 | 1.00 | 28.53 | O |
| ATOM | 3221 | N | LYS | D | 78 | 46.139 | 41.344 | 46.851 | 1.00 | 22.27 | N |
| ATOM | 3222 | CA | LYS | D | 78 | 46.692 | 42.534 | 46.222 | 1.00 | 21.32 | C |
| ATOM | 3223 | C | LYS | D | 78 | 45.654 | 43.318 | 45.471 | 1.00 | 19.56 | C |
| ATOM | 3224 | O | LYS | D | 78 | 45.786 | 44.524 | 45.417 | 1.00 | 22.75 | O |
| ATOM | 3225 | CB | LYS | D | 78 | 47.807 | 42.270 | 45.230 | 1.00 | 23.87 | C |
| ATOM | 3226 | CG | LYS | D | 78 | 49.036 | 41.600 | 45.795 | 1.00 | 30.71 | C |
| ATOM | 3227 | CD | LYS | D | 78 | 50.269 | 41.917 | 44.947 | 1.00 | 37.30 | C |
| ATOM | 3228 | CE | LYS | D | 78 | 51.317 | 40.799 | 45.004 | 1.00 | 40.34 | C |
| ATOM | 3229 | NZ | LYS | D | 78 | 50.843 | 39.671 | 44.214 | 1.00 | 44.85 | N |
| ATOM | 3230 | N | LEU | D | 79 | 44.634 | 42.714 | 44.882 | 1.00 | 18.00 | N |
| ATOM | 3231 | CA | LEU | D | 79 | 43.570 | 43.462 | 44.247 | 1.00 | 16.42 | C |
| ATOM | 3232 | C | LEU | D | 79 | 42.696 | 44.124 | 45.273 | 1.00 | 18.98 | C |
| ATOM | 3233 | O | LEU | D | 79 | 42.215 | 45.218 | 45.035 | 1.00 | 21.86 | O |
| ATOM | 3234 | CB | LEU | D | 79 | 42.687 | 42.543 | 43.451 | 1.00 | 13.71 | C |
| ATOM | 3235 | CG | LEU | D | 79 | 43.383 | 41.746 | 42.358 | 1.00 | 13.81 | C |
| ATOM | 3236 | CD1 | LEU | D | 79 | 42.294 | 41.091 | 41.522 | 1.00 | 14.16 | C |
| ATOM | 3237 | CD2 | LEU | D | 79 | 44.240 | 42.627 | 41.462 | 1.00 | 11.49 | C |
| ATOM | 3238 | N | VAL | D | 80 | 42.438 | 43.524 | 46.430 | 1.00 | 19.01 | N |
| ATOM | 3239 | CA | VAL | D | 80 | 41.624 | 44.124 | 47.462 | 1.00 | 20.11 | C |
| ATOM | 3240 | C | VAL | D | 80 | 42.369 | 45.343 | 47.920 | 1.00 | 21.57 | C |
| ATOM | 3241 | O | VAL | D | 80 | 41.759 | 46.389 | 47.987 | 1.00 | 25.14 | O |
| ATOM | 3242 | CB | VAL | D | 80 | 41.480 | 43.093 | 48.603 | 1.00 | 22.94 | C |
| ATOM | 3243 | CG1 | VAL | D | 80 | 40.920 | 43.647 | 49.896 | 1.00 | 25.85 | C |
| ATOM | 3244 | CG2 | VAL | D | 80 | 40.511 | 42.003 | 48.246 | 1.00 | 20.39 | C |
| ATOM | 3245 | N | ASN | D | 81 | 43.678 | 45.313 | 48.167 | 1.00 | 24.08 | N |
| ATOM | 3246 | CA | ASN | D | 81 | 44.375 | 46.498 | 48.626 | 1.00 | 23.59 | C |
| ATOM | 3247 | C | ASN | D | 81 | 44.363 | 47.632 | 47.620 | 1.00 | 26.17 | C |

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FIGURE 8A-67

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3368 | CG | PHE | D | 110 | 28.993 | 39.305 | 37.265 | 1.00 | 18.38 | C |
| ATOM | 3369 | CD1 | PHE | D | 110 | 28.573 | 39.743 | 36.029 | 1.00 | 19.11 | C |
| ATOM | 3370 | CD2 | PHE | D | 110 | 28.633 | 39.977 | 38.408 | 1.00 | 16.78 | C |
| ATOM | 3371 | CE1 | PHE | D | 110 | 27.802 | 40.874 | 35.946 | 1.00 | 16.73 | C |
| ATOM | 3372 | CE2 | PHE | D | 110 | 27.850 | 41.103 | 38.321 | 1.00 | 18.17 | C |
| ATOM | 3373 | CZ | PHE | D | 110 | 27.445 | 41.553 | 37.081 | 1.00 | 21.53 | C |
| ATOM | 3374 | N | THR | D | 111 | 30.425 | 35.107 | 36.216 | 1.00 | 15.24 | N |
| ATOM | 3375 | CA | THR | D | 111 | 31.539 | 34.192 | 36.176 | 1.00 | 14.72 | C |
| ATOM | 3376 | C | THR | D | 111 | 32.811 | 34.994 | 36.443 | 1.00 | 12.40 | C |
| ATOM | 3377 | O | THR | D | 111 | 32.752 | 36.218 | 36.400 | 1.00 | 13.27 | C |
| ATOM | 3378 | CB | THR | D | 111 | 31.579 | 33.435 | 34.828 | 1.00 | 17.68 | O |
| ATOM | 3379 | OG1 | THR | D | 111 | 31.630 | 34.415 | 33.809 | 1.00 | 17.12 | C |
| ATOM | 3380 | CG2 | THR | D | 111 | 30.451 | 32.446 | 34.621 | 1.00 | 14.81 | O |
| ATOM | 3381 | N | PRO | D | 112 | 33.974 | 34.412 | 36.757 | 1.00 | 12.31 | C |
| ATOM | 3382 | CA | PRO | D | 112 | 35.219 | 35.126 | 36.935 | 1.00 | 11.10 | C |
| ATOM | 3383 | C | PRO | D | 112 | 35.594 | 36.046 | 35.783 | 1.00 | 14.02 | C |
| ATOM | 3384 | O | PRO | D | 112 | 35.884 | 37.215 | 36.011 | 1.00 | 13.17 | O |
| ATOM | 3385 | CB | PRO | D | 112 | 36.189 | 33.965 | 37.074 | 1.00 | 9.39 | C |
| ATOM | 3386 | CG | PRO | D | 112 | 35.413 | 32.952 | 37.854 | 1.00 | 7.72 | C |
| ATOM | 3387 | CD | PRO | D | 112 | 34.151 | 32.972 | 37.061 | 1.00 | 11.01 | C |
| ATOM | 3388 | N | GLU | D | 113 | 35.611 | 35.572 | 34.517 | 1.00 | 16.22 | N |
| ATOM | 3389 | CA | GLU | D | 113 | 35.905 | 36.456 | 33.395 | 1.00 | 16.17 | C |
| ATOM | 3390 | C | GLU | D | 113 | 35.026 | 37.679 | 33.272 | 1.00 | 13.99 | C |
| ATOM | 3391 | O | GLU | D | 113 | 35.508 | 38.761 | 32.985 | 1.00 | 15.09 | C |
| ATOM | 3392 | CB | GLU | D | 113 | 35.913 | 35.703 | 32.092 | 1.00 | 17.91 | O |
| ATOM | 3393 | CG | GLU | D | 113 | 34.636 | 34.985 | 31.713 | 1.00 | 19.43 | C |
| ATOM | 3394 | CD | GLU | D | 113 | 34.621 | 34.539 | 30.277 | 1.00 | 22.34 | C |
| ATOM | 3395 | OE1 | GLU | D | 113 | 35.652 | 34.599 | 29.608 | 1.00 | 23.91 | O |
| ATOM | 3396 | OE2 | GLU | D | 113 | 33.558 | 34.139 | 29.810 | 1.00 | 24.64 | O |
| ATOM | 3397 | N | GLU | D | 114 | 33.747 | 37.539 | 33.559 | 1.00 | 14.85 | N |
| ATOM | 3398 | CA | GLU | D | 114 | 32.837 | 38.649 | 33.596 | 1.00 | 15.81 | C |
| ATOM | 3399 | C | GLU | D | 114 | 33.063 | 39.567 | 34.769 | 1.00 | 15.50 | C |
| ATOM | 3400 | O | GLU | D | 114 | 33.085 | 40.783 | 34.557 | 1.00 | 15.87 | O |
| ATOM | 3401 | CB | GLU | D | 114 | 31.402 | 38.208 | 33.707 | 1.00 | 19.13 | C |
| ATOM | 3402 | CG | GLU | D | 114 | 30.883 | 37.422 | 32.539 | 1.00 | 21.49 | C |
| ATOM | 3403 | CD | GLU | D | 114 | 29.605 | 36.642 | 32.816 | 1.00 | 24.09 | C |
| ATOM | 3404 | OE1 | GLU | D | 114 | 29.017 | 36.697 | 33.897 | 1.00 | 26.51 | O |
| ATOM | 3405 | OE2 | GLU | D | 114 | 29.185 | 35.937 | 31.907 | 1.00 | 29.29 | O |
| ATOM | 3406 | N | PHE | D | 115 | 33.204 | 39.041 | 35.990 | 1.00 | 13.99 | N |
| ATOM | 3407 | CA | PHE | D | 115 | 33.464 | 39.892 | 37.125 | 1.00 | 12.83 | C |
| ATOM | 3408 | C | PHE | D | 115 | 34.753 | 40.667 | 36.905 | 1.00 | 13.21 | C |
| ATOM | 3409 | O | PHE | D | 115 | 34.827 | 41.855 | 37.193 | 1.00 | 14.99 | O |
| ATOM | 3410 | CB | PHE | D | 115 | 33.650 | 39.018 | 38.359 | 1.00 | 10.89 | C |
| ATOM | 3411 | CG | PHE | D | 115 | 33.982 | 39.867 | 39.569 | 1.00 | 11.83 | C |
| ATOM | 3412 | CD1 | PHE | D | 115 | 32.951 | 40.361 | 40.344 | 1.00 | 12.60 | C |
| ATOM | 3413 | CD2 | PHE | D | 115 | 35.296 | 40.133 | 39.917 | 1.00 | 14.96 | C |
| ATOM | 3414 | CE1 | PHE | D | 115 | 33.251 | 41.093 | 41.480 | 1.00 | 12.59 | C |
| ATOM | 3415 | CE2 | PHE | D | 115 | 35.605 | 40.892 | 41.033 | 1.00 | 13.04 | C |
| ATOM | 3416 | CZ | PHE | D | 115 | 34.560 | 41.373 | 41.810 | 1.00 | 14.57 | C |
| ATOM | 3417 | N | PHE | D | 116 | 35.833 | 40.025 | 36.477 | 1.00 | 15.07 | N |
| ATOM | 3418 | CA | PHE | D | 116 | 37.102 | 40.718 | 36.297 | 1.00 | 13.94 | C |
| ATOM | 3419 | C | PHE | D | 116 | 37.181 | 41.563 | 35.036 | 1.00 | 15.79 | C |
| ATOM | 3420 | O | PHE | D | 116 | 38.014 | 42.455 | 34.965 | 1.00 | 16.79 | O |
| ATOM | 3421 | CB | PHE | D | 116 | 38.273 | 39.775 | 36.373 | 1.00 | 13.55 | C |
| ATOM | 3422 | CG | PHE | D | 116 | 38.548 | 39.261 | 37.759 | 1.00 | 10.27 | C |
| ATOM | 3423 | CD1 | PHE | D | 116 | 39.105 | 40.100 | 38.692 | 1.00 | 12.82 | C |
| ATOM | 3424 | CD2 | PHE | D | 116 | 38.143 | 37.990 | 38.132 | 1.00 | 11.47 | C |
| ATOM | 3425 | CE1 | PHE | D | 116 | 39.169 | 39.689 | 40.025 | 1.00 | 14.46 | C |
| ATOM | 3426 | CE2 | PHE | D | 116 | 38.216 | 37.584 | 39.457 | 1.00 | 10.67 | C |
| ATOM | 3427 | CZ | PHE | D | 116 | 38.709 | 38.439 | 40.407 | 1.00 | 11.80 | C |

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FIGURE 8A-68

| | | | | | | | | | | | |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 3428 | N | ARG | D | 117 | 36.361 | 41.405 | 34.011 | 1.00 | 16.57 | N |
| ATOM | 3429 | CA | ARG | D | 117 | 36.293 | 42.421 | 32.990 | 1.00 | 20.64 | C |
| ATOM | 3430 | C | ARG | D | 117 | 35.668 | 43.700 | 33.548 | 1.00 | 22.51 | C |
| ATOM | 3431 | O | ARG | D | 117 | 36.089 | 44.803 | 33.174 | 1.00 | 23.89 | O |
| ATOM | 3432 | CB | ARG | D | 117 | 35.446 | 41.879 | 31.860 | 1.00 | 26.52 | C |
| ATOM | 3433 | CG | ARG | D | 117 | 35.518 | 42.709 | 30.598 | 1.00 | 31.58 | C |
| ATOM | 3434 | CD | ARG | D | 117 | 34.496 | 42.146 | 29.640 | 1.00 | 35.05 | C |
| ATOM | 3435 | NE | ARG | D | 117 | 34.394 | 43.021 | 28.483 | 1.00 | 38.58 | C |
| ATOM | 3436 | CZ | ARG | D | 117 | 33.828 | 42.656 | 27.326 | 1.00 | 37.56 | N |
| ATOM | 3437 | NH1 | ARG | D | 117 | 33.169 | 41.506 | 27.170 | 1.00 | 33.95 | C |
| ATOM | 3438 | NH2 | ARG | D | 117 | 34.002 | 43.473 | 26.286 | 1.00 | 37.95 | N |
| ATOM | 3439 | N | ILE | D | 118 | 34.656 | 43.594 | 34.445 | 1.00 | 22.03 | N |
| ATOM | 3440 | CA | ILE | D | 118 | 34.052 | 44.753 | 35.121 | 1.00 | 19.63 | C |
| ATOM | 3441 | C | ILE | D | 118 | 35.047 | 45.368 | 36.086 | 1.00 | 19.88 | C |
| ATOM | 3442 | O | ILE | D | 118 | 35.183 | 46.586 | 36.085 | 1.00 | 23.21 | O |
| ATOM | 3443 | CB | ILE | D | 118 | 32.781 | 44.357 | 35.874 | 1.00 | 20.68 | C |
| ATOM | 3444 | CG1 | ILE | D | 118 | 31.691 | 43.843 | 34.951 | 1.00 | 19.48 | C |
| ATOM | 3445 | CG2 | ILE | D | 118 | 32.255 | 45.562 | 36.619 | 1.00 | 20.52 | C |
| ATOM | 3446 | CD1 | ILE | D | 118 | 30.567 | 43.143 | 35.727 | 1.00 | 18.63 | C |
| ATOM | 3447 | N | PHE | D | 119 | 35.741 | 44.577 | 36.908 | 1.00 | 16.07 | N |
| ATOM | 3448 | CA | PHE | D | 119 | 36.853 | 45.059 | 37.683 | 1.00 | 15.72 | C |
| ATOM | 3449 | C | PHE | D | 119 | 37.853 | 45.894 | 36.880 | 1.00 | 17.75 | C |
| ATOM | 3450 | O | PHE | D | 119 | 38.208 | 47.006 | 37.267 | 1.00 | 20.22 | O |
| ATOM | 3451 | CB | PHE | D | 119 | 37.545 | 43.866 | 38.359 | 1.00 | 12.02 | C |
| ATOM | 3452 | CG | PHE | D | 119 | 38.822 | 44.222 | 39.100 | 1.00 | 13.89 | C |
| ATOM | 3453 | CD1 | PHE | D | 119 | 38.760 | 44.766 | 40.389 | 1.00 | 14.47 | C |
| ATOM | 3454 | CD2 | PHE | D | 119 | 40.057 | 44.030 | 38.492 | 1.00 | 10.48 | C |
| ATOM | 3455 | CE1 | PHE | D | 119 | 39.944 | 45.148 | 41.032 | 1.00 | 13.14 | C |
| ATOM | 3456 | CE2 | PHE | D | 119 | 41.219 | 44.387 | 39.149 | 1.00 | 10.95 | C |
| ATOM | 3457 | CZ | PHE | D | 119 | 41.163 | 44.965 | 40.405 | 1.00 | 10.47 | C |
| ATOM | 3458 | N | ASN | D | 120 | 38.349 | 45.343 | 35.779 | 1.00 | 18.18 | N |
| ATOM | 3459 | CA | ASN | D | 120 | 39.325 | 45.994 | 34.955 | 1.00 | 18.15 | C |
| ATOM | 3460 | C | ASN | D | 120 | 38.709 | 47.263 | 34.387 | 1.00 | 20.79 | C |
| ATOM | 3461 | O | ASN | D | 120 | 39.348 | 48.303 | 34.408 | 1.00 | 22.36 | O |
| ATOM | 3462 | CB | ASN | D | 120 | 39.805 | 45.078 | 33.812 | 1.00 | 18.05 | C |
| ATOM | 3463 | CG | ASN | D | 120 | 40.849 | 44.026 | 34.137 | 1.00 | 17.71 | C |
| ATOM | 3464 | OD1 | ASN | D | 120 | 41.770 | 44.210 | 34.918 | 1.00 | 21.36 | O |
| ATOM | 3465 | ND2 | ASN | D | 120 | 40.765 | 42.860 | 33.538 | 1.00 | 17.03 | N |
| ATOM | 3466 | N | ARG | D | 121 | 37.463 | 47.256 | 33.941 | 1.00 | 22.71 | N |
| ATOM | 3467 | CA | ARG | D | 121 | 36.824 | 48.438 | 33.431 | 1.00 | 24.59 | C |
| ATOM | 3468 | C | ARG | D | 121 | 36.703 | 49.523 | 34.494 | 1.00 | 27.41 | C |
| ATOM | 3469 | O | ARG | D | 121 | 36.971 | 50.683 | 34.192 | 1.00 | 30.49 | O |
| ATOM | 3470 | CB | ARG | D | 121 | 35.468 | 47.993 | 32.953 | 1.00 | 26.42 | C |
| ATOM | 3471 | CG | ARG | D | 121 | 34.608 | 49.156 | 32.549 | 1.00 | 33.46 | C |
| ATOM | 3472 | CD | ARG | D | 121 | 34.760 | 49.641 | 31.105 | 1.00 | 37.32 | C |
| ATOM | 3473 | NE | ARG | D | 121 | 34.149 | 50.962 | 30.882 | 1.00 | 39.99 | C |
| ATOM | 3474 | CZ | ARG | D | 121 | 32.836 | 51.217 | 31.020 | 1.00 | 39.01 | N |
| ATOM | 3475 | NH1 | ARG | D | 121 | 31.955 | 50.306 | 31.426 | 1.00 | 37.27 | C |
| ATOM | 3476 | NH2 | ARG | D | 121 | 32.392 | 52.439 | 30.747 | 1.00 | 40.47 | N |
| ATOM | 3477 | N | SER | D | 122 | 36.364 | 49.186 | 35.754 | 1.00 | 28.07 | N |
| ATOM | 3478 | CA | SER | D | 122 | 36.147 | 50.153 | 36.820 | 1.00 | 24.66 | C |
| ATOM | 3479 | C | SER | D | 122 | 37.455 | 50.758 | 37.250 | 1.00 | 25.38 | C |
| ATOM | 3480 | O | SER | D | 122 | 37.536 | 51.971 | 37.401 | 1.00 | 24.85 | O |
| ATOM | 3481 | CB | SER | D | 122 | 35.452 | 49.505 | 37.983 | 1.00 | 20.76 | C |
| ATOM | 3482 | OG | SER | D | 122 | 34.236 | 48.886 | 37.591 | 1.00 | 19.10 | O |
| ATOM | 3483 | N | ILE | D | 123 | 38.513 | 49.954 | 37.389 | 1.00 | 28.58 | N |
| ATOM | 3484 | CA | ILE | D | 123 | 39.853 | 50.468 | 37.718 | 1.00 | 31.03 | C |
| ATOM | 3485 | C | ILE | D | 123 | 40.396 | 51.464 | 36.684 | 1.00 | 33.54 | C |
| ATOM | 3486 | O | ILE | D | 123 | 40.998 | 52.471 | 37.040 | 1.00 | 33.54 | O |
| ATOM | 3487 | CB | ILE | D | 123 | 40.821 | 49.267 | 38.041 | 1.00 | 31.69 | O |

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FIGURE 8A-69

| | | | | | | | | | | | |
|--------|------|-----|-----|---|------|--------|--------|--------|------|-------|----|
| ATOM | 3488 | CG1 | ILE | D | 123 | 40.899 | 48.877 | 39.544 | 1.00 | 30.91 | C |
| ATOM | 3489 | CG2 | ILE | D | 123 | 42.262 | 49.504 | 37.583 | 1.00 | 31.27 | C |
| ATOM | 3490 | CD1 | ILE | D | 123 | 39.609 | 48.826 | 40.377 | 1.00 | 31.19 | C |
| ATOM | 3491 | N | ASP | D | 124 | 40.123 | 51.244 | 35.395 | 1.00 | 36.80 | N |
| ATOM | 3492 | CA | ASP | D | 124 | 40.562 | 52.125 | 34.333 | 1.00 | 38.72 | C |
| ATOM | 3493 | C | ASP | D | 124 | 39.846 | 53.455 | 34.353 | 1.00 | 39.18 | C |
| ATOM | 3494 | O | ASP | D | 124 | 40.487 | 54.491 | 34.186 | 1.00 | 39.94 | O |
| ATOM | 3495 | CB | ASP | D | 124 | 40.383 | 51.461 | 32.981 | 1.00 | 42.50 | C |
| ATOM | 3496 | CG | ASP | D | 124 | 40.847 | 52.342 | 31.828 | 1.00 | 47.69 | C |
| ATOM | 3497 | OD1 | ASP | D | 124 | 42.058 | 52.554 | 31.646 | 1.00 | 50.62 | C |
| ATOM | 3498 | OD2 | ASP | D | 124 | 39.972 | 52.837 | 31.116 | 1.00 | 51.18 | O |
| ATOM | 3499 | N | ALA | D | 125 | 38.538 | 53.440 | 34.590 | 1.00 | 39.43 | N |
| ATOM | 3500 | CA | ALA | D | 125 | 37.731 | 54.649 | 34.586 | 1.00 | 41.04 | C |
| ATOM | 3501 | C | ALA | D | 125 | 38.028 | 55.640 | 35.712 | 1.00 | 44.24 | C |
| ATOM | 3502 | O | ALA | D | 125 | 37.580 | 56.792 | 35.729 | 1.00 | 46.63 | O |
| ATOM | 3503 | CB | ALA | D | 125 | 36.289 | 54.232 | 34.688 | 1.00 | 37.89 | C |
| ATOM | 3504 | N | PHE | D | 126 | 38.795 | 55.189 | 36.693 | 1.00 | 47.55 | N |
| ATOM | 3505 | CA | PHE | D | 126 | 39.342 | 56.063 | 37.709 | 1.00 | 52.08 | C |
| ATOM | 3506 | C | PHE | D | 126 | 40.409 | 57.058 | 37.208 | 1.00 | 55.06 | C |
| ATOM | 3507 | O | PHE | D | 126 | 40.531 | 58.167 | 37.751 | 1.00 | 57.33 | O |
| ATOM | 3508 | CB | PHE | D | 126 | 39.877 | 55.182 | 38.838 | 1.00 | 51.90 | C |
| ATOM | 3509 | CG | PHE | D | 126 | 39.154 | 55.489 | 40.124 | 1.00 | 50.92 | C |
| ATOM | 3510 | CD1 | PHE | D | 126 | 39.155 | 56.780 | 40.620 | 1.00 | 52.88 | C |
| ATOM | 3511 | CD2 | PHE | D | 126 | 38.437 | 54.505 | 40.745 | 1.00 | 50.11 | C |
| ATOM | 3512 | CE1 | PHE | D | 126 | 38.390 | 57.105 | 41.721 | 1.00 | 54.34 | C |
| ATOM | 3513 | CE2 | PHE | D | 126 | 37.688 | 54.827 | 41.851 | 1.00 | 52.08 | C |
| ATOM | 3514 | CZ | PHE | D | 126 | 37.653 | 56.117 | 42.336 | 1.00 | 53.64 | C |
| ATOM | 3515 | N | LYS | D | 127 | 41.187 | 56.667 | 36.177 | 1.00 | 56.75 | N |
| ATOM | 3516 | CA | LYS | D | 127 | 42.055 | 57.566 | 35.420 | 1.00 | 57.29 | C |
| ATOM | 3517 | C | LYS | D | 127 | 41.257 | 58.229 | 34.273 | 1.00 | 58.91 | C |
| ATOM | 3518 | O | LYS | D | 127 | 41.376 | 57.826 | 33.098 | 1.00 | 60.03 | O |
| ATOM | 3519 | CB | LYS | D | 127 | 43.225 | 56.735 | 34.882 | 1.00 | 56.61 | C |
| TER | 3521 | | LYS | D | 127 | | | | | | |
| HETATM | 3522 | CA | CA | | 1021 | 34.563 | 32.796 | 27.927 | 1.00 | 28.47 | CA |
| HETATM | 3523 | CA | CA | | 1022 | 29.874 | 41.216 | 51.866 | 1.00 | 42.93 | CA |
| HETATM | 3524 | CA | CA | | 1023 | 46.453 | 8.630 | 31.415 | 1.00 | 34.99 | CA |
| HETATM | 3525 | OH2 | 1PE | | 1 | 18.016 | 39.096 | 31.870 | 1.00 | 54.04 | O |
| HETATM | 3526 | C12 | 1PE | | 1 | 19.233 | 39.467 | 31.241 | 1.00 | 52.50 | C |
| HETATM | 3527 | C22 | 1PE | | 1 | 20.344 | 39.764 | 32.285 | 1.00 | 52.87 | C |
| HETATM | 3528 | OH3 | 1PE | | 1 | 21.455 | 40.455 | 31.657 | 1.00 | 50.81 | O |
| HETATM | 3529 | C13 | 1PE | | 1 | 21.887 | 42.392 | 30.182 | 1.00 | 41.29 | C |
| HETATM | 3530 | C23 | 1PE | | 1 | 20.971 | 41.737 | 31.213 | 1.00 | 45.45 | C |
| HETATM | 3531 | OH4 | 1PE | | 1 | 23.085 | 42.870 | 30.757 | 1.00 | 37.80 | C |
| HETATM | 3532 | C14 | 1PE | | 1 | 24.265 | 44.731 | 31.534 | 1.00 | 39.00 | C |
| HETATM | 3533 | C24 | 1PE | | 1 | 22.866 | 44.120 | 31.391 | 1.00 | 35.49 | C |
| HETATM | 3534 | OH5 | 1PE | | 1 | 25.158 | 43.676 | 31.917 | 1.00 | 39.07 | O |
| HETATM | 3535 | C15 | 1PE | | 1 | 27.396 | 42.942 | 31.976 | 1.00 | 36.51 | C |
| HETATM | 3536 | C25 | 1PE | | 1 | 26.476 | 44.138 | 32.222 | 1.00 | 37.63 | C |
| HETATM | 3537 | OH6 | 1PE | | 1 | 26.797 | 41.817 | 32.602 | 1.00 | 37.94 | O |
| HETATM | 3538 | C16 | 1PE | | 1 | 28.795 | 40.537 | 32.878 | 1.00 | 44.86 | C |
| HETATM | 3539 | C26 | 1PE | | 1 | 27.405 | 40.589 | 32.251 | 1.00 | 38.90 | C |
| HETATM | 3540 | OH7 | 1PE | | 1 | 29.817 | 40.999 | 31.987 | 1.00 | 53.59 | O |
| HETATM | 3541 | O | HOH | | 1024 | 36.890 | 32.430 | 27.721 | 1.00 | 24.58 | O |
| HETATM | 3542 | O | HOH | | 1025 | 35.049 | 30.934 | 29.322 | 1.00 | 27.97 | O |
| HETATM | 3543 | O | HOH | | 1026 | 31.347 | 42.865 | 52.839 | 1.00 | 31.45 | O |
| HETATM | 3544 | O | HOH | | 1027 | 44.819 | 10.251 | 32.056 | 1.00 | 31.08 | O |
| HETATM | 3545 | O | HOH | | 1028 | 47.508 | 7.695 | 33.365 | 1.00 | 35.15 | O |
| HETATM | 3546 | O | HOH | | 1029 | 48.695 | 9.256 | 30.957 | 1.00 | 29.22 | O |
| HETATM | 3547 | O | HOH | | 1105 | 33.704 | 13.935 | 20.986 | 1.00 | 32.21 | O |
| HETATM | 3548 | O | HOH | | 1106 | 22.707 | 17.800 | 13.006 | 1.00 | 51.74 | O |

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FIGURE 8A-70

| | | | | | | | | | |
|-------------|---|-----|------|--------|---------|--------|------|-------|---|
| HETATM 3549 | O | HOH | 1107 | 25.589 | 22.952 | 23.068 | 1.00 | 38.86 | O |
| HETATM 3550 | O | HOH | 1108 | 20.410 | 17.104 | 15.299 | 1.00 | 29.07 | O |
| HETATM 3551 | O | HOH | 1109 | 26.763 | 8.355 | 29.315 | 1.00 | 19.21 | O |
| HETATM 3552 | O | HOH | 1110 | 25.744 | 13.365 | 30.461 | 1.00 | 32.06 | O |
| HETATM 3553 | O | HOH | 1111 | 27.532 | 6.721 | 32.848 | 1.00 | 38.65 | O |
| HETATM 3554 | O | HOH | 1112 | 18.245 | 18.266 | 16.629 | 1.00 | 28.39 | O |
| HETATM 3555 | O | HOH | 1113 | 23.260 | 14.366 | 29.164 | 1.00 | 21.00 | O |
| HETATM 3556 | O | HOH | 1114 | 15.116 | 22.225 | 22.815 | 1.00 | 19.32 | O |
| HETATM 3557 | O | HOH | 1115 | 15.033 | 21.355 | 35.696 | 1.00 | 38.95 | O |
| HETATM 3558 | O | HOH | 1116 | 20.651 | 6.306 | 35.427 | 1.00 | 25.08 | O |
| HETATM 3559 | O | HOH | 1117 | 15.267 | 18.912 | 37.475 | 1.00 | 41.62 | O |
| HETATM 3560 | O | HOH | 1118 | 13.693 | 14.872 | 13.312 | 1.00 | 29.91 | O |
| HETATM 3561 | O | HOH | 1119 | 10.257 | 20.310 | 28.411 | 1.00 | 19.75 | O |
| HETATM 3562 | O | HOH | 1120 | 17.034 | 0.246 | 35.599 | 1.00 | 32.81 | O |
| HETATM 3563 | O | HOH | 1121 | 6.051 | 17.933 | 31.202 | 1.00 | 21.61 | O |
| HETATM 3564 | O | HOH | 1122 | 4.997 | 14.576 | 24.993 | 1.00 | 33.94 | O |
| HETATM 3565 | O | HOH | 1123 | 0.916 | 19.643 | 30.618 | 1.00 | 37.91 | O |
| HETATM 3566 | O | HOH | 1124 | 5.906 | 11.136 | 30.408 | 1.00 | 46.39 | O |
| HETATM 3567 | O | HOH | 1125 | 6.559 | 5.604 | 30.508 | 1.00 | 37.39 | O |
| HETATM 3568 | O | HOH | 1126 | 8.033 | 4.439 | 28.006 | 1.00 | 43.67 | O |
| HETATM 3569 | O | HCH | 1127 | 5.753 | 3.756 | 33.445 | 1.00 | 43.48 | O |
| HETATM 3570 | O | HOH | 1128 | 44.059 | 26.360 | 36.277 | 1.00 | 22.42 | O |
| HETATM 3571 | O | HOH | 1129 | 34.421 | 31.639 | 20.635 | 1.00 | 57.58 | O |
| HETATM 3572 | O | HOH | 1130 | 50.215 | 13.426 | 34.211 | 1.00 | 31.74 | O |
| HETATM 3573 | O | HOH | 1132 | 22.455 | 45.496 | 39.519 | 1.00 | 46.16 | O |
| HETATM 3574 | O | HOH | 1133 | 13.246 | 35.686 | 8.764 | 1.00 | 63.66 | O |
| HETATM 3575 | O | HOH | 1134 | 34.029 | 21.538 | 54.154 | 1.00 | 48.71 | O |
| HETATM 3576 | O | HOH | 1135 | 46.505 | 41.139 | 53.506 | 1.00 | 25.80 | O |
| HETATM 3577 | O | HOH | 1136 | 14.868 | 40.514 | 7.810 | 1.00 | 46.95 | O |
| HETATM 3578 | O | HOH | 1138 | 37.977 | 45.274 | 53.726 | 1.00 | 41.75 | O |
| HETATM 3579 | O | HOH | 1139 | 10.511 | 41.610 | 30.508 | 1.00 | 54.06 | O |
| HETATM 3580 | O | HOH | 1140 | 21.928 | 44.651 | 36.769 | 1.00 | 27.65 | O |
| HETATM 3581 | O | HOH | 1141 | 9.657 | 38.390 | 31.085 | 1.00 | 36.52 | O |
| HETATM 3582 | O | HOH | 1142 | 35.556 | 55.905 | 31.455 | 1.00 | 33.05 | O |
| HETATM 3583 | O | HOH | 1143 | 52.337 | 31.433 | 47.975 | 1.00 | 42.15 | O |
| HETATM 3584 | O | HCH | 1144 | 32.915 | 38.699 | 23.494 | 1.00 | 40.84 | O |
| HETATM 3585 | O | HOH | 1145 | 29.548 | 21.469 | 24.434 | 1.00 | 44.50 | O |
| HETATM 3586 | O | HOH | 1146 | 26.181 | 34.331 | 29.823 | 1.00 | 34.71 | O |
| HETATM 3587 | O | HOH | 1147 | 39.069 | 5.943 | 33.085 | 1.00 | 53.70 | O |
| HETATM 3588 | O | HOH | 1148 | 34.970 | 24.222 | 52.427 | 1.00 | 40.12 | O |
| HETATM 3589 | O | HOH | 1149 | 59.825 | 24.478 | 48.580 | 1.00 | 40.98 | O |
| HETATM 3590 | O | HOH | 1150 | 28.412 | 33.531 | 47.673 | 1.00 | 44.44 | O |
| HETATM 3591 | O | HOH | 1151 | 25.454 | 33.933 | 32.960 | 1.00 | 35.88 | O |
| HETATM 3592 | O | HOH | 1152 | 41.875 | 59.115 | 53.350 | 1.00 | 51.54 | O |
| HETATM 3593 | O | HOH | 1153 | 45.977 | 17.661 | 29.654 | 1.00 | 48.44 | O |
| HETATM 3594 | O | HOH | 1154 | 16.374 | 19.854 | 15.198 | 1.00 | 26.92 | O |
| HETATM 3595 | O | HOH | 1156 | 2.909 | 45.550 | 9.710 | 1.00 | 33.50 | O |
| HETATM 3596 | O | HOH | 1157 | 27.955 | 42.970 | 52.054 | 1.00 | 42.09 | O |
| HETATM 3597 | O | HOH | 1158 | 18.671 | 28.692 | 31.947 | 1.00 | 31.92 | O |
| HETATM 3598 | O | HOH | 1160 | 31.097 | 11.069 | 39.837 | 1.00 | 22.54 | O |
| HETATM 3599 | O | HOH | 1161 | 24.551 | 47.693 | 13.911 | 1.00 | 39.92 | O |
| HETATM 3600 | O | HOH | 1162 | 19.328 | 46.523 | 39.555 | 1.00 | 49.64 | O |
| HETATM 3601 | O | HOH | 1163 | 14.463 | 28.577 | 32.747 | 1.00 | 33.62 | O |
| HETATM 3602 | O | HOH | 1164 | 42.334 | 34.141 | 31.684 | 1.00 | 25.02 | O |
| HETATM 3603 | O | HOH | 1165 | 26.640 | 35.518 | 34.853 | 1.00 | 25.40 | O |
| HETATM 3604 | O | HOH | 1166 | 41.719 | 26.191 | 52.537 | 1.00 | 54.23 | O |
| HETATM 3605 | O | HOH | 1167 | 11.799 | 43.370 | 8.564 | 1.00 | 42.64 | O |
| HETATM 3606 | O | HOH | 1169 | 39.695 | 23.691 | 29.775 | 1.00 | 46.55 | O |
| HETATM 3607 | O | HOH | 1170 | 25.519 | -10.203 | 13.390 | 1.00 | 29.39 | O |
| HETATM 3608 | O | HOH | 1172 | 15.639 | 30.378 | 9.410 | 1.00 | 35.98 | O |

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FIGURE 8A-71

| | | | | | | | | | |
|-------------|---|-----|------|--------|--------|--------|------|-------|---|
| HETATM 3609 | O | HOH | 1173 | 26.042 | 53.508 | 19.228 | 1.00 | 35.35 | O |
| HETATM 3610 | O | HOH | 1174 | 16.723 | 43.317 | 9.437 | 1.00 | 70.54 | O |
| HETATM 3611 | O | HOH | 1175 | 11.039 | 27.202 | 31.989 | 1.00 | 35.23 | O |
| HETATM 3612 | O | HOH | 1176 | 26.492 | 54.880 | 14.660 | 1.00 | 45.35 | O |
| HETATM 3613 | O | HOH | 1177 | 48.739 | 5.603 | 40.080 | 1.00 | 46.72 | O |
| HETATM 3614 | O | HOH | 1179 | 38.452 | 10.611 | 56.410 | 1.00 | 33.18 | O |
| HETATM 3615 | O | HOH | 1180 | 25.173 | 41.020 | 50.981 | 1.00 | 37.80 | O |
| HETATM 3616 | O | HOH | 1181 | 26.009 | 21.500 | 26.306 | 1.00 | 37.33 | O |
| HETATM 3617 | O | HOH | 1185 | 32.901 | 61.354 | 32.974 | 1.00 | 47.36 | O |
| HETATM 3618 | O | HOH | 1186 | 49.199 | 44.404 | 48.616 | 1.00 | 55.72 | O |
| HETATM 3619 | O | HOH | 1187 | 28.401 | 31.064 | 46.621 | 1.00 | 25.46 | O |
| HETATM 3620 | O | HOH | 1189 | 50.488 | 34.252 | 43.662 | 1.00 | 27.11 | O |
| HETATM 3621 | O | HOH | 1190 | 25.015 | 38.231 | 32.413 | 1.00 | 46.20 | O |
| HETATM 3622 | O | HOH | 1191 | 13.328 | 45.647 | 6.880 | 1.00 | 50.19 | O |
| HETATM 3623 | O | HOH | 1192 | 9.102 | 28.582 | 30.815 | 1.00 | 28.84 | O |
| HETATM 3624 | O | HOH | 1194 | 16.216 | 53.125 | 18.778 | 1.00 | 20.19 | O |
| HETATM 3625 | O | HOH | 1195 | 48.924 | 37.778 | 50.511 | 1.00 | 41.81 | O |
| HETATM 3626 | O | HOH | 1196 | 29.151 | 29.120 | 42.414 | 1.00 | 25.51 | O |
| HETATM 3627 | O | HOH | 1197 | 10.760 | 56.327 | 24.871 | 1.00 | 25.61 | O |
| HETATM 3628 | O | HOH | 1198 | 19.161 | 31.540 | 33.429 | 1.00 | 41.50 | O |
| HETATM 3629 | O | HOH | 1201 | 31.584 | 19.545 | 39.778 | 1.00 | 41.14 | O |
| HETATM 3630 | O | HOH | 1202 | 31.499 | 33.130 | 31.243 | 1.00 | 30.94 | O |
| HETATM 3631 | O | HOH | 1203 | 33.475 | 31.251 | 32.729 | 1.00 | 30.16 | O |
| HETATM 3632 | O | HOH | 1204 | 25.323 | 26.251 | 24.066 | 1.00 | 29.38 | O |
| HETATM 3633 | O | HOH | 1205 | 18.912 | 50.780 | 14.345 | 1.00 | 28.88 | O |
| HETATM 3634 | O | HOH | 1206 | 28.562 | 46.055 | 22.818 | 1.00 | 37.71 | O |
| HETATM 3635 | O | HOH | 1207 | 31.212 | 15.396 | 37.505 | 1.00 | 38.29 | O |
| HETATM 3636 | O | HOH | 1208 | 21.188 | 13.368 | 44.376 | 1.00 | 22.37 | O |
| HETATM 3637 | O | HOH | 1209 | 17.682 | 38.715 | 10.160 | 1.00 | 31.02 | O |
| HETATM 3638 | O | HOH | 1210 | 50.214 | 11.867 | 37.111 | 1.00 | 50.09 | O |
| HETATM 3639 | O | HOH | 1212 | 28.768 | 41.646 | 47.276 | 1.00 | 22.25 | O |
| HETATM 3640 | O | HOH | 1214 | 49.993 | 18.233 | 34.806 | 1.00 | 44.55 | O |
| HETATM 3641 | O | HOH | 1215 | 32.815 | 34.522 | 46.504 | 1.00 | 35.13 | O |
| HETATM 3642 | O | HOH | 1216 | 39.893 | 28.328 | 41.896 | 1.00 | 12.01 | O |
| HETATM 3643 | O | HOH | 1217 | 15.338 | 26.949 | 28.916 | 1.00 | 11.70 | O |
| HETATM 3644 | O | HOH | 1218 | 35.548 | 32.617 | 33.681 | 1.00 | 18.33 | O |
| HETATM 3645 | O | HOH | 1219 | 39.368 | 28.656 | 34.414 | 1.00 | 16.49 | O |
| HETATM 3646 | O | HOH | 1220 | 10.631 | 22.205 | 16.485 | 1.00 | 23.48 | O |
| HETATM 3647 | O | HOH | 1221 | 38.404 | 33.931 | 29.548 | 1.00 | 20.31 | O |
| HETATM 3648 | O | HOH | 1222 | 29.170 | 43.940 | 45.652 | 1.00 | 17.85 | O |
| HETATM 3649 | O | HOH | 1223 | 16.493 | 28.977 | 30.383 | 1.00 | 19.55 | O |
| HETATM 3650 | O | HOH | 1224 | 50.201 | 26.750 | 43.278 | 1.00 | 23.76 | O |
| HETATM 3651 | O | HOH | 1225 | 38.642 | 25.017 | 49.298 | 1.00 | 24.48 | O |
| HETATM 3652 | O | HOH | 1226 | 22.132 | 37.260 | 38.648 | 1.00 | 21.90 | O |
| HETATM 3653 | O | HOH | 1227 | 39.985 | 27.256 | 49.971 | 1.00 | 19.31 | O |
| HETATM 3654 | O | HOH | 1228 | 46.680 | 26.589 | 41.727 | 1.00 | 24.34 | O |
| HETATM 3655 | O | HOH | 1229 | 45.783 | 30.693 | 47.582 | 1.00 | 25.33 | O |
| HETATM 3656 | O | HOH | 1230 | 37.132 | 23.521 | 50.764 | 1.00 | 25.39 | O |
| HETATM 3657 | O | HOH | 1231 | 37.666 | 45.416 | 31.269 | 1.00 | 22.37 | O |
| HETATM 3658 | O | HOH | 1232 | 12.017 | 34.217 | 29.751 | 1.00 | 24.35 | O |
| HETATM 3659 | O | HOH | 1233 | 26.995 | 45.967 | 27.617 | 1.00 | 23.52 | O |
| HETATM 3660 | O | HOH | 1234 | 26.536 | 25.536 | 28.250 | 1.00 | 29.21 | O |
| HETATM 3661 | O | HOH | 1235 | 25.412 | 37.399 | 29.161 | 1.00 | 27.51 | O |
| HETATM 3662 | O | HOH | 1236 | 37.339 | 31.390 | 35.413 | 1.00 | 25.38 | O |
| HETATM 3663 | O | HOH | 1237 | 49.870 | 32.179 | 49.678 | 1.00 | 25.92 | O |
| HETATM 3664 | O | HOH | 1238 | 22.061 | 39.616 | 17.387 | 1.00 | 15.04 | O |
| HETATM 3665 | O | HOH | 1239 | 14.228 | 24.366 | 29.787 | 1.00 | 22.47 | O |
| HETATM 3666 | O | HOH | 1240 | 23.022 | 47.566 | 29.327 | 1.00 | 39.50 | O |
| HETATM 3667 | O | HOH | 1241 | 21.098 | 32.679 | 17.559 | 1.00 | 35.09 | O |
| HETATM 3668 | O | HOH | 1242 | 23.864 | 37.449 | 16.707 | 1.00 | 37.28 | O |

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FIGURE 8A-72

| | | | | | | | | | | |
|--------|------|---|-----|------|--------|--------|--------|------|-------|---|
| HETATM | 3669 | O | HOH | 1243 | 32.934 | 17.639 | 38.491 | 1.00 | 30.00 | 0 |
| HETATM | 3670 | O | HOH | 1244 | 30.081 | 39.275 | 47.475 | 1.00 | 27.25 | 0 |
| HETATM | 3671 | O | HOH | 1245 | 40.219 | 10.507 | 54.210 | 1.00 | 42.36 | 0 |
| HETATM | 3672 | O | HOH | 1246 | 20.198 | 57.839 | 14.584 | 1.00 | 26.12 | 0 |
| HETATM | 3673 | O | HOH | 1247 | 22.701 | 31.034 | 19.118 | 1.00 | 26.32 | 0 |
| HETATM | 3674 | O | HOH | 1248 | 50.529 | 25.000 | 51.117 | 1.00 | 16.36 | 0 |
| HETATM | 3675 | O | HOH | 1249 | 27.308 | 27.122 | 38.575 | 1.00 | 29.98 | 0 |
| HETATM | 3676 | O | HOH | 1250 | 41.664 | 46.630 | 31.018 | 1.00 | 29.42 | 0 |
| HETATM | 3677 | O | HOH | 1251 | 27.841 | 34.202 | 44.699 | 1.00 | 37.98 | 0 |
| HETATM | 3678 | O | HOH | 1252 | 28.946 | 26.204 | 44.341 | 1.00 | 51.94 | 0 |
| HETATM | 3679 | O | HOH | 1253 | 26.643 | 43.795 | 23.560 | 1.00 | 23.03 | 0 |
| HETATM | 3680 | O | HOH | 1254 | 52.894 | 25.886 | 44.095 | 1.00 | 33.52 | 0 |
| HETATM | 3681 | O | HOH | 1255 | 42.339 | 26.613 | 55.952 | 1.00 | 36.97 | 0 |
| HETATM | 3682 | O | HOH | 1256 | 48.804 | 2.432 | 50.876 | 1.00 | 36.59 | 0 |
| HETATM | 3683 | O | HOH | 1257 | 51.244 | 18.531 | 40.805 | 1.00 | 33.51 | 0 |
| HETATM | 3684 | O | HOH | 1260 | 49.903 | 39.828 | 48.137 | 1.00 | 44.77 | 0 |
| HETATM | 3685 | O | HOH | 1261 | 45.720 | 4.638 | 32.384 | 1.00 | 54.41 | 0 |
| HETATM | 3686 | O | HOH | 1262 | 32.871 | 29.567 | 30.088 | 1.00 | 39.72 | 0 |
| HETATM | 3687 | O | HOH | 1263 | 23.890 | 51.918 | 23.175 | 1.00 | 37.61 | 0 |
| HETATM | 3688 | O | HOH | 1264 | 13.550 | 26.049 | 31.905 | 1.00 | 33.45 | 0 |
| HETATM | 3689 | O | HOH | 1266 | 10.689 | 31.547 | 31.432 | 1.00 | 47.94 | 0 |
| HETATM | 3690 | O | HOH | 1269 | 26.086 | -7.425 | 31.507 | 1.00 | 39.58 | 0 |
| HETATM | 3691 | O | HOH | 1271 | 22.022 | 54.673 | 22.853 | 1.00 | 37.03 | 0 |
| HETATM | 3692 | O | HOH | 1274 | 28.901 | 24.308 | 41.027 | 1.00 | 41.39 | 0 |
| HETATM | 3693 | O | HOH | 1276 | 45.609 | -2.697 | 31.603 | 1.00 | 49.62 | 0 |
| HETATM | 3694 | O | HOH | 1277 | 9.649 | 26.708 | 34.475 | 1.00 | 36.02 | 0 |
| HETATM | 3695 | O | HOH | 1279 | 21.970 | 8.818 | 36.303 | 1.00 | 45.69 | 0 |
| HETATM | 3696 | O | HOH | 1280 | 7.956 | 56.039 | 27.031 | 1.00 | 55.41 | 0 |
| HETATM | 3697 | O | HOH | 1281 | 15.342 | 17.025 | 12.461 | 1.00 | 55.13 | 0 |
| HETATM | 3698 | O | HOH | 1284 | 12.862 | 44.437 | 3.810 | 1.00 | 49.95 | 0 |
| HETATM | 3699 | O | HOH | 1286 | 34.675 | 64.010 | 47.159 | 1.00 | 47.97 | 0 |
| HETATM | 3700 | O | HOH | 1287 | 41.049 | 11.857 | 30.681 | 1.00 | 29.94 | 0 |
| HETATM | 3701 | O | HOH | 1288 | 34.457 | 19.302 | 55.855 | 1.00 | 47.88 | 0 |
| HETATM | 3702 | O | HOH | 1289 | 28.546 | 31.433 | 28.564 | 1.00 | 47.71 | 0 |
| HETATM | 3703 | O | HOH | 1291 | 33.220 | 60.645 | 39.548 | 1.00 | 52.03 | 0 |
| HETATM | 3704 | O | HOH | 1292 | 30.910 | 54.312 | 27.471 | 1.00 | 48.06 | 0 |
| HETATM | 3705 | O | HOH | 1293 | 23.058 | 27.656 | 32.358 | 1.00 | 45.02 | 0 |
| HETATM | 3706 | O | HOH | 1294 | 28.377 | 27.865 | 25.772 | 1.00 | 37.73 | 0 |
| HETATM | 3707 | O | HOH | 1295 | 17.851 | 13.033 | 47.051 | 1.00 | 31.43 | 0 |
| HETATM | 3708 | O | HOH | 1297 | 22.435 | 24.151 | 33.420 | 1.00 | 39.38 | 0 |
| HETATM | 3709 | O | HOH | 1298 | 29.292 | 20.833 | 37.423 | 1.00 | 52.78 | 0 |
| HETATM | 3710 | O | HOH | 1299 | 26.196 | 40.554 | 47.655 | 1.00 | 52.83 | 0 |
| HETATM | 3711 | O | HOH | 1300 | 6.687 | 28.384 | 34.247 | 1.00 | 45.71 | 0 |
| HETATM | 3712 | O | HOH | 1303 | 41.624 | 1.272 | 27.661 | 1.00 | 61.55 | 0 |
| HETATM | 3713 | O | HOH | 1306 | 24.865 | 48.368 | 49.108 | 1.00 | 53.05 | 0 |
| HETATM | 3714 | O | HOH | 1308 | 43.375 | 33.196 | 54.115 | 1.00 | 34.68 | 0 |
| HETATM | 3715 | O | HOH | 1309 | 24.941 | 16.106 | 28.105 | 1.00 | 27.22 | 0 |
| HETATM | 3716 | O | HOH | 1310 | 48.767 | 36.362 | 53.067 | 1.00 | 39.18 | 0 |
| HETATM | 3717 | O | HOH | 1311 | 0.897 | 25.934 | 24.841 | 1.00 | 47.80 | 0 |
| HETATM | 3718 | O | HOH | 1312 | 41.531 | 54.883 | 30.082 | 1.00 | 37.92 | 0 |
| HETATM | 3719 | O | HOH | 1315 | 32.370 | 19.055 | 31.177 | 1.00 | 43.71 | 0 |
| HETATM | 3720 | O | HOH | 1316 | 19.469 | 15.072 | 45.662 | 1.00 | 48.16 | 0 |
| HETATM | 3721 | O | HOH | 1321 | 10.144 | 48.734 | 5.731 | 1.00 | 39.11 | 0 |
| HETATM | 3722 | O | HOH | 1322 | 29.076 | 56.977 | 42.203 | 1.00 | 46.38 | 0 |
| HETATM | 3723 | O | HOH | 1326 | 42.727 | 8.091 | 54.610 | 1.00 | 56.42 | 0 |
| HETATM | 3724 | O | HOH | 1330 | 41.316 | 20.071 | 29.052 | 1.00 | 39.86 | 0 |
| HETATM | 3725 | O | HOH | 1331 | 16.596 | 27.837 | 34.825 | 1.00 | 50.15 | 0 |
| HETATM | 3726 | O | HOH | 1332 | 19.903 | 45.162 | 47.256 | 1.00 | 52.33 | 0 |
| HETATM | 3727 | O | HOH | 1333 | 40.238 | -8.133 | 39.062 | 1.00 | 41.11 | 0 |
| HETATM | 3728 | O | HOH | 1335 | 32.007 | 37.168 | 46.170 | 1.00 | 43.84 | 0 |

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FIGURE 8A-73

| | | | | | | | | | | |
|--------|------|---|-----|------|--------|---------|--------|------|-------|---|
| HETATM | 3729 | O | HOH | 1337 | 8.866 | 32.982 | 29.638 | 1.00 | 51.57 | 0 |
| HETATM | 3730 | O | HOH | 1339 | 35.650 | 46.023 | 29.211 | 1.00 | 40.99 | 0 |
| HETATM | 3731 | O | HOH | 1340 | 52.825 | 32.335 | 38.756 | 1.00 | 50.57 | 0 |
| HETATM | 3732 | O | HOH | 1341 | 36.938 | 51.807 | 31.314 | 1.00 | 45.30 | 0 |
| HETATM | 3733 | O | HOH | 1342 | 18.790 | 42.705 | 33.580 | 1.00 | 43.47 | 0 |
| HETATM | 3734 | O | HOH | 1344 | 22.819 | 36.661 | 11.619 | 1.00 | 46.70 | 0 |
| HETATM | 3735 | O | HOH | 1345 | 19.465 | 28.669 | 34.714 | 1.00 | 39.89 | 0 |
| HETATM | 3736 | O | HOH | 1347 | 40.179 | 23.790 | 53.530 | 1.00 | 47.43 | 0 |
| HETATM | 3737 | O | HOH | 1353 | 3.487 | 36.484 | 13.806 | 1.00 | 40.41 | 0 |
| HETATM | 3738 | O | HOH | 1360 | 31.223 | 4.884 | 34.089 | 1.00 | 30.96 | 0 |
| HETATM | 3739 | O | HOH | 1361 | 19.647 | 3.819 | 14.444 | 1.00 | 26.16 | 0 |
| HETATM | 3740 | O | HOH | 1364 | 12.171 | -3.712 | 34.829 | 1.00 | 52.07 | 0 |
| HETATM | 3741 | O | HOH | 1366 | 14.715 | 10.503 | 15.414 | 1.00 | 47.98 | 0 |
| HETATM | 3742 | O | HOH | 1370 | 3.284 | 18.073 | 30.684 | 1.00 | 39.22 | 0 |
| HETATM | 3743 | O | HOH | 1371 | 16.114 | 12.267 | 13.222 | 1.00 | 41.79 | 0 |
| HETATM | 3744 | O | HOH | 1374 | 26.710 | -10.158 | 28.570 | 1.00 | 46.72 | 0 |
| HETATM | 3745 | O | HOH | 1376 | 13.842 | 2.095 | 17.391 | 1.00 | 51.23 | 0 |
| HETATM | 3746 | O | HOH | 1377 | 23.624 | 18.176 | 26.993 | 1.00 | 46.55 | 0 |
| HETATM | 3747 | O | HOH | 1378 | 17.679 | 9.897 | 14.906 | 1.00 | 29.42 | 0 |
| HETATM | 3748 | O | HOH | 1380 | 21.173 | -2.881 | 15.825 | 1.00 | 44.25 | 0 |
| HETATM | 3749 | O | HOH | 1381 | 25.990 | 6.184 | 14.411 | 1.00 | 40.98 | 0 |
| HETATM | 3750 | O | HOH | 1382 | 25.475 | 8.938 | 15.031 | 1.00 | 40.93 | 0 |
| HETATM | 3751 | O | HOH | 1384 | 27.045 | 17.549 | 12.911 | 1.00 | 44.46 | 0 |
| HETATM | 3752 | O | HOH | 1387 | 15.174 | -5.506 | 13.111 | 1.00 | 43.09 | 0 |
| HETATM | 3753 | O | HOH | 1388 | 3.093 | 25.580 | 28.841 | 1.00 | 47.33 | 0 |
| HETATM | 3754 | O | HOH | 1389 | 43.833 | 14.822 | 32.665 | 1.00 | 30.09 | 0 |
| HETATM | 3755 | O | HOH | 1390 | 27.283 | 3.257 | 16.277 | 1.00 | 28.50 | 0 |
| HETATM | 3756 | O | HOH | 1391 | 31.590 | 8.583 | 17.790 | 1.00 | 31.43 | 0 |
| HETATM | 3757 | O | HOH | 1392 | 28.183 | 8.699 | 15.618 | 1.00 | 37.69 | 0 |
| HETATM | 3758 | O | HOH | 1393 | 24.599 | 3.854 | 15.072 | 1.00 | 40.30 | 0 |
| HETATM | 3759 | O | HOH | 1404 | 39.148 | 30.436 | 32.035 | 1.00 | 17.64 | 0 |
| HETATM | 3760 | O | HOH | 1405 | 0.837 | 22.245 | 22.324 | 1.00 | 55.83 | 0 |
| HETATM | 3761 | O | HOH | 1406 | 29.799 | 34.134 | 27.910 | 1.00 | 28.75 | 0 |
| HETATM | 3762 | O | HOH | 1407 | 18.445 | 6.222 | 44.059 | 1.00 | 53.71 | 0 |
| HETATM | 3763 | O | HOH | 1409 | 30.392 | 39.323 | 25.039 | 1.00 | 34.89 | 0 |
| HETATM | 3764 | O | HOH | 1410 | 18.490 | 9.793 | 47.086 | 1.00 | 48.51 | 0 |
| HETATM | 3765 | O | HOH | 1411 | 13.220 | 32.748 | 8.629 | 1.00 | 49.26 | 0 |
| HETATM | 3766 | O | HOH | 1412 | 49.361 | 20.100 | 32.438 | 1.00 | 43.65 | 0 |
| HETATM | 3767 | O | HOH | 1414 | 51.855 | 33.864 | 41.242 | 1.00 | 64.26 | 0 |
| HETATM | 3768 | O | HOH | 1418 | 47.727 | 41.100 | 41.717 | 1.00 | 35.47 | 0 |
| HETATM | 3769 | O | HOH | 1419 | 24.466 | 54.548 | 43.747 | 1.00 | 53.28 | 0 |
| HETATM | 3770 | O | HOH | 1420 | 5.934 | 30.983 | 8.318 | 1.00 | 45.39 | 0 |
| HETATM | 3771 | O | HOH | 1421 | 32.399 | -4.433 | 42.259 | 1.00 | 41.31 | 0 |
| HETATM | 3772 | O | HOH | 1422 | 3.024 | 40.996 | 27.927 | 1.00 | 42.40 | 0 |
| HETATM | 3773 | O | HOH | 1424 | 36.321 | -0.489 | 35.913 | 1.00 | 41.12 | 0 |
| HETATM | 3774 | O | HOH | 1428 | 16.200 | 42.165 | 4.789 | 1.00 | 62.98 | 0 |
| HETATM | 3775 | O | HOH | 1429 | 4.930 | 40.213 | 24.269 | 1.00 | 53.41 | 0 |
| HETATM | 3776 | O | HOH | 1430 | 7.506 | 9.248 | 13.243 | 1.00 | 51.74 | 0 |
| HETATM | 3777 | O | HOH | 1434 | 16.093 | 51.978 | 11.936 | 1.00 | 39.24 | 0 |
| HETATM | 3778 | O | HOH | 1437 | 32.063 | 21.866 | 31.547 | 1.00 | 49.87 | 0 |
| HETATM | 3779 | O | HOH | 1438 | 54.621 | 26.247 | 29.147 | 1.00 | 48.62 | 0 |
| HETATM | 3780 | O | HOH | 1440 | 4.318 | 19.369 | 8.919 | 1.00 | 47.53 | 0 |
| HETATM | 3781 | O | HOH | 1441 | 5.136 | 2.358 | 29.831 | 1.00 | 44.25 | 0 |
| HETATM | 3782 | O | HOH | 1443 | 2.076 | 24.174 | 15.211 | 1.00 | 53.91 | 0 |
| HETATM | 3783 | O | HOH | 1444 | 15.474 | 42.729 | 30.690 | 1.00 | 38.63 | 0 |
| HETATM | 3784 | O | HOH | 1446 | 34.955 | 9.442 | 53.656 | 1.00 | 51.40 | 0 |
| HETATM | 3785 | O | HOH | 1447 | 28.597 | 17.387 | 31.041 | 1.00 | 40.53 | 0 |
| HETATM | 3786 | O | HOH | 1454 | 34.884 | -9.534 | 12.912 | 1.00 | 33.84 | 0 |
| HETATM | 3787 | O | HOH | 1455 | 56.971 | 31.610 | 49.136 | 1.00 | 44.36 | 0 |
| HETATM | 3788 | O | HOH | 1456 | 29.676 | 11.548 | 53.175 | 1.00 | 41.64 | 0 |

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FIGURE 8A-74

| | | | | | | | | | | |
|--------|------|------|------|------|--------|--------|--------|------|-------|---|
| HETATM | 3789 | O | HOH | 1457 | 46.713 | 47.217 | 35.996 | 1.00 | 51.75 | O |
| HETATM | 3790 | O | HOH | 1458 | 22.556 | 3.172 | 12.871 | 1.00 | 35.99 | O |
| HETATM | 3791 | O | HOH | 1459 | 42.572 | 42.347 | 52.583 | 1.00 | 55.24 | O |
| HETATM | 3792 | O | HOH | 1461 | 0.573 | 13.064 | 16.484 | 1.00 | 44.57 | O |
| HETATM | 3793 | O | HOH | 1462 | 50.467 | 6.260 | 32.228 | 1.00 | 46.40 | O |
| HETATM | 3794 | O | HOH | 1463 | 6.167 | 47.337 | 5.349 | 1.00 | 53.27 | O |
| HETATM | 3795 | O | HOH | 1464 | 24.604 | -9.866 | 26.249 | 1.00 | 43.72 | O |
| HETATM | 3796 | O | HOH | 1466 | 22.806 | 17.220 | 45.236 | 1.00 | 61.41 | O |
| HETATM | 3797 | O | HOH | 1506 | 25.441 | 49.608 | 19.993 | 1.00 | 33.89 | O |
| HETATM | 3798 | O | HOH | 1507 | 39.709 | -9.399 | 16.482 | 1.00 | 30.44 | O |
| HETATM | 3799 | O | HOH | 1509 | 9.926 | 24.411 | 36.529 | 1.00 | 37.21 | O |
| HETATM | 3800 | O | HOH | 1515 | 34.731 | 28.232 | 28.355 | 1.00 | 37.81 | O |
| HETATM | 3801 | O | HOH | 1518 | 44.323 | 37.583 | 28.523 | 1.00 | 44.08 | O |
| HETATM | 3802 | O | HOH | 1519 | 30.194 | -0.768 | 45.229 | 1.00 | 40.11 | O |
| HETATM | 3803 | O | HOH | 1521 | 42.425 | 48.375 | 34.242 | 1.00 | 50.42 | O |
| HETATM | 3804 | O | HOH | 1523 | 12.185 | 2.224 | 34.335 | 1.00 | 56.22 | O |
| CONECT | 109 | 108 | 110 | 119 | | | | | | |
| CONECT | 119 | 109 | 120 | | | | | | | |
| CONECT | 120 | 119 | 121 | 123 | | | | | | |
| CONECT | 121 | 120 | 122 | 127 | | | | | | |
| CONECT | 122 | 121 | | | | | | | | |
| CONECT | 123 | 120 | 124 | | | | | | | |
| CONECT | 124 | 123 | 125 | | | | | | | |
| CONECT | 125 | 124 | 126 | | | | | | | |
| CONECT | 126 | 125 | | | | | | | | |
| CONECT | 127 | 121 | 128 | | | | | | | |
| CONECT | 187 | 186 | 188 | 189 | | | | | | |
| CONECT | 189 | 187 | 190 | | | | | | | |
| CONECT | 190 | 189 | 191 | 193 | | | | | | |
| CONECT | 191 | 190 | 192 | 197 | | | | | | |
| CONECT | 192 | 191 | | | | | | | | |
| CONECT | 193 | 190 | 194 | | | | | | | |
| CONECT | 194 | 193 | 195 | | | | | | | |
| CONECT | 195 | 194 | 196 | | | | | | | |
| CONECT | 196 | 195 | | | | | | | | |
| CONECT | 197 | 191 | 198 | | | | | | | |
| CONECT | 248 | 247 | 905 | | | | | | | |
| CONECT | 279 | 278 | 280 | 286 | | | | | | |
| CONECT | 286 | 279 | 287 | | | | | | | |
| CONECT | 287 | 286 | 288 | 290 | | | | | | |
| CONECT | 288 | 287 | 289 | 294 | | | | | | |
| CONECT | 289 | 288 | | | | | | | | |
| CONECT | 290 | 287 | 291 | | | | | | | |
| CONECT | 291 | 290 | 292 | | | | | | | |
| CONECT | 292 | 291 | 293 | | | | | | | |
| CONECT | 293 | 292 | | | | | | | | |
| CONECT | 294 | 288 | 295 | | | | | | | |
| CONECT | 905 | 248 | 904 | | | | | | | |
| CONECT | 1038 | 1037 | 1039 | 1048 | | | | | | |
| CONECT | 1048 | 1038 | 1049 | | | | | | | |
| CONECT | 1049 | 1048 | 1050 | 1052 | | | | | | |
| CONECT | 1050 | 1049 | 1051 | 1056 | | | | | | |
| CONECT | 1051 | 1050 | | | | | | | | |
| CONECT | 1052 | 1049 | 1053 | | | | | | | |
| CONECT | 1053 | 1052 | 1054 | | | | | | | |
| CONECT | 1054 | 1053 | 1055 | | | | | | | |
| CONECT | 1055 | 1054 | | | | | | | | |
| CONECT | 1056 | 1050 | 1057 | | | | | | | |
| CONECT | 1116 | 1115 | 1117 | 1118 | | | | | | |
| CONECT | 1118 | 1116 | 1119 | | | | | | | |

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FIGURE 8A-75

CONECT 1119 1118 1120 1122
CONECT 1120 1119 1121 1126
CONECT 1121 1120
CONECT 1122 1119 1123
CONECT 1123 1122 1124
CONECT 1124 1123 1125
CONECT 1125 1124
CONECT 1126 1120 1127
CONECT 1177 1176 1874
CONECT 1208 1207 1209 1215
CONECT 1215 1208 1216
CONECT 1216 1215 1217 1219
CONECT 1217 1216 1218 1223
CONECT 1218 1217
CONECT 1219 1216 1220
CONECT 1220 1219 1221
CONECT 1221 1220 1222
CONECT 1222 1221
CONECT 1223 1217 1224
CONECT 1874 1177 1873
CONECT 1987 1986 1988 1997
CONECT 1997 1987 1998
CONECT 1998 1997 1999 2001
CONECT 1999 1998 2000 2005
CONECT 2000 1999
CONECT 2001 1998 2002
CONECT 2002 2001 2003
CONECT 2003 2002 2004
CONECT 2004 2003
CONECT 2005 1999 2006
CONECT 2065 2064 2066 2067
CONECT 2067 2065 2068
CONECT 2068 2067 2069 2071
CONECT 2069 2068 2070 2075
CONECT 2070 2069
CONECT 2071 2068 2072
CONECT 2072 2071 2073
CONECT 2073 2072 2074
CONECT 2074 2073
CONECT 2075 2069 2076
CONECT 2154 2153 2155 2161
CONECT 2161 2154 2162
CONECT 2162 2161 2163 2165
CONECT 2163 2162 2164 2169
CONECT 2164 2163
CONECT 2165 2162 2166
CONECT 2166 2165 2167
CONECT 2167 2166 2168
CONECT 2168 2167
CONECT 2169 2163 2170
CONECT 2813 2812 2814 2823
CONECT 2823 2813 2824
CONECT 2824 2823 2825 2827
CONECT 2825 2824 2826 2831
CONECT 2826 2825
CONECT 2827 2824 2828
CONECT 2828 2827 2829
CONECT 2829 2828 2830
CONECT 2830 2829
CONECT 2831 2825 2832

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FIGURE 8A-76

CONECT 2891 2890 2892 2893
CONECT 2893 2891 2894
CONECT 2894 2893 2895 2897
CONECT 2895 2894 2896 2901
CONECT 2896 2895
CONECT 2897 2894 2898
CONECT 2898 2897 2899
CONECT 2899 2898 2900
CONECT 2900 2899
CONECT 2901 2895 2902
CONECT 2983 2982 2984 2990
CONECT 2990 2983 2991
CONECT 2991 2990 2992 2994
CONECT 2992 2991 2993 2998
CONECT 2993 2992
CONECT 2994 2991 2995
CONECT 2995 2994 2996
CONECT 2996 2995 2997
CONECT 2997 2996
CONECT 2998 2992 2999
CONECT 3522 3541 3542
CONECT 3524 3544 3545 3546
CONECT 3525 3526
CONECT 3526 3525 3527
CONECT 3527 3526 3528
CONECT 3528 3527 3530
CONECT 3529 3530 3531
CONECT 3530 3528 3529
CONECT 3531 3529 3533
CONECT 3532 3533 3534
CONECT 3533 3531 3532
CONECT 3534 3532 3536
CONECT 3535 3536 3537
CONECT 3536 3534 3535
CONECT 3537 3535 3539
CONECT 3538 3539 3540
CONECT 3539 3537 3538
CONECT 3540 3538
CONECT 3541 3522
CONECT 3542 3522
CONECT 3544 3524
CONECT 3545 3524
CONECT 3546 3524
MASTER 301 0 16 19 8 0 0 27 3796 4 147 84
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